Unit 12

Partial differential equations

Introduction

A **partial differential equation** is an equation relating a dependent variable and two or more independent variables through *partial derivatives* of the dependent variable. An example is

Partial derivatives were introduced in Unit 7.

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = e^{-(x^2+y^2)},$$

in which the dependent variable u is a function $u(x, y)$ of two independent variables, x and y.

Differential equations have played a very important role in the module so far. But until now, all the differential equations that you have solved have had just one independent variable, and contained *ordinary* derivatives with respect to that independent variable. Such equations are often called *ordinary differential equations* when it is necessary to distinguish them from partial differential equations. For many of the systems that we want to model, ordinary differential equations are inadequate because the states of the system can be specified only in terms of two – or even more – independent variables. When we are trying to describe the way in which such a system changes, we are inevitably led to consider partial differential equations.

Ordinary differential equations are the subject of Units 2, 3, 6 and 13.

Partial differential equations and fields

Much of the third book of this module was concerned with scalar and vector fields. You will be familiar with the idea that a scalar field can describe how a quantity such as temperature varies throughout space, and that this field is described by a function – for example, $\theta(x, y, z, t)$ might be the temperature at position (x, y, z) and time t. But we always regarded the fields as 'given' quantities: we specified the functions describing the fields, without discussing how these functions can be obtained.

In this unit, temperature is denoted by the symbol θ.

In fact, the laws of nature that determine scalar and vector fields are often formulated as partial differential equations. This makes the study of partial differential equations a key skill for anyone who wants to understand physical sciences at a quantitative level.

Having studied Units 1 and 2, you will appreciate that solving differential equations can be difficult, and that analytic solutions are not always available. It should be no surprise that partial differential equations are typically harder to solve. However, it turns out that many of the most important partial differential equations can be solved by the *method of separation of variables*, which is covered in this unit.

This unit concentrates on two examples of partial differential equations, namely the *wave equation* and the *diffusion equation*. Both of these equations describe how a scalar quantity (u, say) varies in space and time.

We concentrate on the simplest situation, the *one-dimensional* case, where there is only one coordinate, x, for the space dependence, and time is represented by t.

Wave equation and diffusion equation

The one-dimensional form of the **wave equation** is

$$\frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2}, \tag{1}$$

where c is a positive constant called the **wave speed**.

The one-dimensional **diffusion equation** is

$$\frac{\partial u}{\partial t} = D\,\frac{\partial^2 u}{\partial x^2}, \tag{2}$$

where D is a positive constant called the **diffusion coefficient**.

The diffusion equation is also known as the **heat equation**. The contexts in which these equations arise will be described later in the unit.

Classification of partial differential equations

There are systematic ways of classifying partial differential equations, based on the classification of ordinary differential equations. You do not need to remember the definitions, but you should be aware of the terminology because you may meet it in more advanced courses.

- The *order* of a partial differential equation is the order of the highest derivative that occurs in it.
- A partial differential equation is *linear* if all terms that contain the dependent variable are proportional to the dependent variable, or one of its partial derivatives, but not both.
- A linear partial differential equation is *homogeneous* if there are no terms that are solely functions of the independent variables.

In this unit we deal only with *second-order linear homogeneous partial differential equations*. From these definitions you can see that both the wave equation (1) and the diffusion equation (2) are examples. By contrast, the partial differential equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - \frac{\partial^2 u}{\partial x^2} = \sin(x+t)$$

is non-linear because of the term that is a product of u and $\partial u/\partial x$, and inhomogeneous because the term $\sin(x+t)$ does not contain u. Equations of this type are beyond the scope of this unit.

Study guide

Section 1 introduces the wave equation and considers how it is used to describe the vibrations of a plucked guitar string. The wave equation is then solved using the method of separation of variables. This very important technique has two main stages. First, we find a set of simple solutions that satisfy the partial differential equation and its boundary conditions. Then we find a linear combination of these simple solutions that satisfies the partial differential equation, its boundary conditions and the given initial conditions. The task of finding the appropriate linear combination in this case makes use of the Fourier methods covered in Unit 11.

Section 2 introduces the diffusion equation, which can be used to model the slow spread of materials, such as the slow spread of a pollutant as it contaminates groundwater. Most of this section is concerned with arguments that justify the form of the diffusion equation. You will not be asked to reproduce these arguments in assignments or in the exam. However, because of the importance of partial differential equations in the physical sciences, it is valuable to see one example of a partial differential equation being derived. The section ends by illustrating the solution of the diffusion equation, again using the method of separation of variables

As well as describing the spread of materials, the diffusion equation also describes the spread of heat. In this context, the diffusion equation is known as the heat equation. The heat equation and some of its solutions are considered in Section 3.

All the solutions considered in Sections 1 to 3 are for cases where the equations describe systems with boundaries. The wave equation and diffusion equation also apply to systems without boundaries, and in these cases useful solutions are available that are not easily obtained by the method of separation of variables. We discuss some useful alternative forms of solution of the wave and diffusion equations in Section 4. However, this section is optional reading.

1 The method of separation of variables

The most important idea that you will learn from this unit is the method of separation of variables for solving linear homogeneous partial differential equations. The wave equation can describe the motion of a plucked string, and we use this as our first example of a partial differential equation that is solved by the method of separation of variables.

1.1 Motion of a plucked guitar string

When asked to imagine a wave, you might think of an ocean wave rolling onto a beach (Figure 1(a)). This type of wave is called a **travelling wave**. But the wave equation can also describe a disturbance that varies in space, and oscillates at each point, but does not move through space. The motion of a guitar string is a good example (Figure 1(b)).

(a) (b)

Figure 1 Two waves: (a) a travelling wave in the ocean; (b) a standing wave on a guitar string

Figure 2 shows a possible motion for such a string. Each coloured curve indicates the shape of the string at a particular instant in time. The dark blue curve corresponds to the earliest time; the green curve to a slightly later time, and so on. The string vibrates 'on the spot', but no wave flows to the left or right, and there are some points (known as **nodes**) where the string remains permanently at rest. Motion such as this is called a **standing wave**.

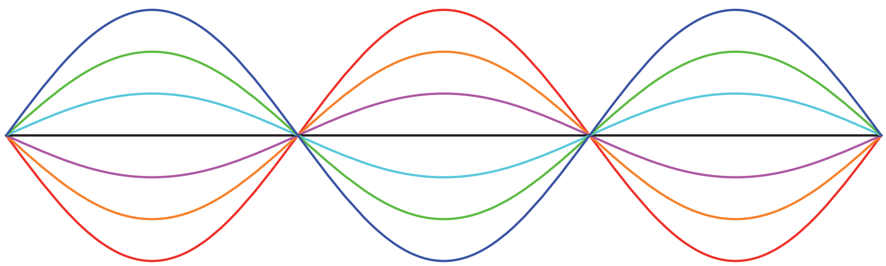


Figure 2 Shapes of a plucked guitar string at a succession of equally-spaced times: the time sequence corresponds to dark blue, green, cyan, black, magenta, orange, red, orange, magenta, black, cyan, green, dark blue, and so on

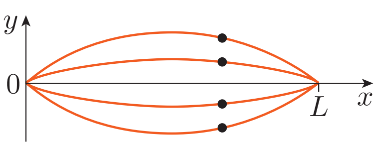
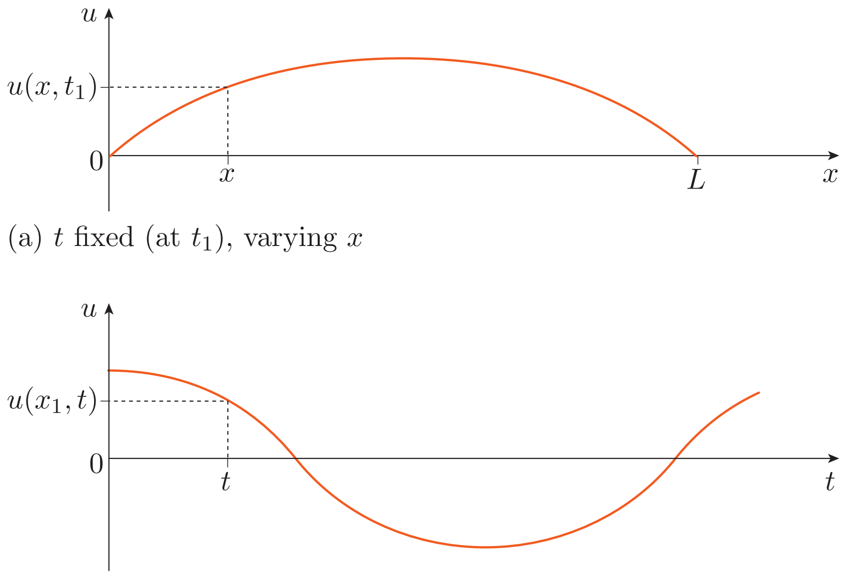


Figure 3 A point on a vibrating string moves up and down

Let us consider the motion of a plucked guitar string in more detail. In its equilibrium state, the string is taut and is anchored at two fixed points separated by a distance L. We take the string to lie along the x-axis, with one end at $x = 0$ and the other at $x = L$. The motion of the string is confined to a plane, which may be taken to be the xy-plane. The motion of each point of the string is assumed to be up and down (or *transverse*) – that is, parallel to the y-axis, with no motion along the x-axis (Figure 3). The transverse displacement of any point on the string is denoted u. The value of u depends on the position x of the point along the string, and also on time t. So we have two independent variables, x and t, and one

dependent variable, u. We say that u is a function of x and t, and write $u = u(x,t)$.

At a fixed time $t = t_1$, the function $u(x,t_1)$ is a function of x alone; this describes the shape of the string at the given time t_1. For a given point on the string, labelled by $x = x_1$, the function $u(x_1,t)$ is a function of t alone; this describes the motion of the given point on the string as time progresses. Figure 4 illustrates both these aspects. Figure 4(a) is a typical graph of $u(x,t_1)$ against x, giving a snapshot of the shape of the string, while Figure 4(b) is a typical graph of $u(x_1,t)$ against t, showing the displacement of a single point on the string as a function of time.



(a) t fixed (at t_1), varying x

(b) x fixed (at x_1), varying t

Figure 4 Graphs of: (a) $u(x,t_1)$ against x, showing the shape of the string at time t_1; (b) $u(x_1,t)$ against t, showing the displacement of a single point on the string as a function of time

In order to describe the motion of the string, we need to find the function $u(x,t)$. Since u depends on both x and t, an equation that models the motion of the string is expected to involve partial derivatives of u with respect to both x and t. The appropriate differential equation for small vibrations of a flexible taut string is the **wave equation**

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2}, \qquad (3)$$

where c is a constant whose value depends on various physical characteristics of the string. This constant is called the **wave speed**, although the reason for this name will become apparent only at the end of this unit. The quantity $\partial^2 u/\partial t^2$ on the right-hand side of equation (3) is the acceleration of a tiny segment of the string. A lengthy analysis shows that the net force acting on this segment is proportional to $\partial^2 u/\partial x^2$. Equation (3) therefore embodies Newton's second law: force is proportional to acceleration. The derivation of the wave equation is not part of this unit.

In fact, c depends on the linear density and tension of the string.

It is easy to check whether or not a function is a solution of a partial differential equation by simply substituting the given function into the given equation, and seeing whether the equation is satisfied. The only difference from the case of an ordinary differential equation is that you have to calculate all the relevant partial derivatives. For example, let us check that

$$u(x,t) = \sin(kx)\cos(kct)$$

is a solution of the wave equation (3) for any constant k. We have

$$\frac{\partial u}{\partial x} = k\cos(kx)\cos(kct), \quad \frac{\partial u}{\partial t} = -kc\sin(kx)\sin(kct),$$
$$\frac{\partial^2 u}{\partial x^2} = -k^2\sin(kx)\cos(kct), \quad \frac{\partial^2 u}{\partial t^2} = -k^2c^2\sin(kx)\cos(kct).$$

So when $u(x,t) = \sin(kx)\cos(kct)$,

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2},$$

and this function is indeed a solution of the wave equation.

Exercise 1

Determine whether $u(x,t) = A\sin(kx)\sin(kct)$, where A and k are real constants, is a solution of the wave equation.

Exercise 2

If the displacement of the string is $u(x,t) = A\sin(kx)\sin(kct)$, find expressions for the displacement and velocity of the string at position x and time $t = 0$. (*Hint*: The velocity at time t is the partial derivative of the displacement with respect to time t.)

Boundary conditions and initial conditions

Initial conditions and boundary conditions were discussed in Unit 3.

Just giving a partial differential equation is never enough to specify a problem completely: some additional information in the form of boundary conditions and/or initial conditions is always required. The boundary conditions and initial conditions appropriate to obtaining a particular solution depend on the context. For example, for the wave equation as a model of the vibrations of a guitar string, we need *two* boundary conditions and *two* initial conditions.

If the string is anchored at $x = 0$ and $x = L$, and we are interested in the motion following the string's release at $t = 0$, then the boundary conditions are

$$u(0,t) = u(L,t) = 0, \quad t \geq 0, \tag{4}$$

corresponding to the string being fixed at its ends.

The initial conditions model the action of releasing the string and setting it in motion. In particular, plucking consists of holding the string in a certain shape, at rest, and then releasing it. If the initial shape of the string is given by a function $f(x)$, then the initial conditions for a plucked string may be specified in the form

$$u(x,0) = f(x), \quad 0 \le x \le L, \tag{5}$$

and

$$\frac{\partial u}{\partial t}(x,0) = 0, \quad 0 \le x \le L. \tag{6}$$

The first initial condition describes the initial shape of the string, while the second corresponds to it being at rest initially. Note that for a partial differential equation, the initial condition is described by a *function* $f(x)$, whereas in the case of an ordinary differential equation an initial condition is described by a number. The initial conditions are often specified piecewise, as in the following example and exercise.

Example 1

A taut string of equilibrium length L is plucked at its midpoint, which is given an initial displacement d, as shown in Figure 5. The string is then released from rest. Write down the initial conditions for the wave equation describing transverse vibrations of this string.

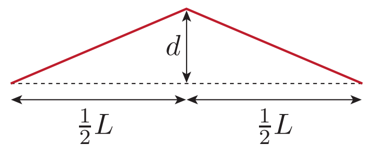


Figure 5 String plucked at its midpoint

Solution

The displacement shown in Figure 5 has two linear sections. The left-hand section has slope $d/(L/2) = 2d/L$ and has the value $u = 0$ at $x = 0$. It is described by the function $u(x) = (2d/L)x$. The right-hand section has slope $-2d/L$ and has the value $u = 0$ at $x = L$. It is described by a linear function of the form

$$u(x) = -\frac{2d}{L}x + C,$$

where C is a constant. Setting $u(L) = 0$ gives $C = 2d$, so the right-hand section is described by the function

$$u(x) = 2d - \frac{2d}{L}x = \frac{2d}{L}(L - x).$$

Hence the initial displacement is given by the piecewise function

$$u(x,0) = \begin{cases} \dfrac{2d}{L}x & \text{for } 0 \le x \le \frac{1}{2}L, \\[2ex] \dfrac{2d}{L}(L-x) & \text{for } \frac{1}{2}L < x \le L. \end{cases}$$

Both parts of this expression give $u(x,0) = d$ at $x = L/2$. This is a useful check.

Because the string is released from rest, the transverse component of the initial velocity is given by

$$\frac{\partial u}{\partial t}(x,0) = 0, \quad 0 \le x \le L.$$

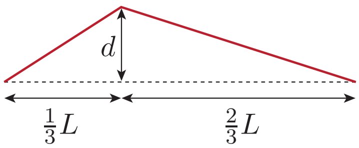


Figure 6 String plucked at a distance $L/3$ from $x = 0$

Exercise 3

A taut string of equilibrium length L is plucked at a point one-third of the way along its length, which is given an initial displacement d, as shown in Figure 6. What are the initial conditions for the wave equation describing transverse vibrations of this string?

We have seen that any function of the form $u(x,t) = \sin(kx)\cos(kct)$ is a solution of the wave equation, for any constant k. In particular, for $k = \pi/L$,

$$u(x,t) = \sin\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi c t}{L}\right) \tag{7}$$

is a solution of the wave equation for transverse vibrations of a taut string, where L is the equilibrium length of the string. This solution also satisfies the boundary conditions (4) and the initial condition $\partial u(x,0)/\partial t = 0$. It describes a special case where the initial displacement of the string is a sinusoidal function, that is, the function $f(x)$ in (5) is $f(x) = \sin(\pi x/L)$.

Exercise 4

Show that the solution given by equation (7) satisfies the boundary conditions

$$u(0,t) = u(L,t) = 0, \quad t \geq 0,$$

and the initial condition

$$\frac{\partial u}{\partial t}(x,0) = 0, \quad 0 \leq x \leq L.$$

Boundary conditions, initial conditions and uniqueness

In general, it may not be clear which boundary and initial conditions are required to go with a given partial differential equation. When solving practical problems, the boundary and initial conditions should contain enough information to determine a unique solution of the partial differential equation. There are mathematical conditions for determining when there is a unique solution. In practice, however, these are rarely used. Usually an understanding of the physics or engineering context is a reliable guide to what sort of initial and boundary conditions are required.

1.2 Separation of variables for the wave equation

We have already said that the most important idea that you will learn from this unit is the method of *separation of variables*. We now apply this method to the wave equation for vibrations of a taut flexible string.

The method described here is not the same as the separation of variables method in Unit 2, which applies to first-order ordinary differential equations.

The method has a number of stages. First, we find some special solutions of the wave equation that satisfy the given boundary conditions. Then we show that linear combinations of these special solutions also satisfy the wave equation. The final stage of the calculation selects the particular linear combination that is needed to ensure that the initial conditions are met. In this subsection, we concentrate on the first stage – finding a set of special solutions of the wave equation from which everything else will be constructed. We require the solutions to satisfy the boundary conditions, but we will not bother with any particular initial conditions at this stage.

The partial differential equation that we wish to solve is the wave equation for vibrations of a taut string:

Sections 2 and 3 will apply the same method to the diffusion equation (also called the heat equation).

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2}, \tag{8}$$

subject to the boundary conditions

$$u(0,t) = u(L,t) = 0, \quad t \geq 0. \tag{9}$$

The first step in the method of separation of variables is to look for solutions of (8) and (9) in the form

$$u(x,t) = X(x)\,T(t), \tag{10}$$

where $X(x)$ is a function of x alone, and $T(t)$ is a function of t alone, so that the variables x and t occur in two separate functions. Note that we are *not* claiming that all the solutions of equation (8) are of this form. We are merely restricting attention to a simple type of solution, in which $u(x,t)$ happens to be the product of a function of x and a function of t. Such solutions are called **product solutions**.

We now prepare to substitute equation (10) into the wave equation. The partial derivative $\partial/\partial x$, with respect to x, acts only on the function $X(x)$, and $\partial/\partial t$ acts only on $T(t)$. Because $X(x)$ and $T(t)$ are both functions of a single variable, their derivatives are written with upright, rather than curly, dees. We therefore have

$$\frac{\partial u}{\partial x} = \frac{dX}{dx}\,T, \quad \frac{\partial u}{\partial t} = X\,\frac{dT}{dt}.$$

Differentiating again gives

$$\frac{\partial^2 u}{\partial x^2} = \frac{d^2X}{dx^2}\,T, \quad \frac{\partial^2 u}{\partial t^2} = X\,\frac{d^2T}{dt^2}.$$

Substituting these second-order partial derivatives into the wave equation then leads to

$$T\,\frac{d^2X}{dx^2} = \frac{1}{c^2}X\,\frac{d^2T}{dt^2}. \tag{11}$$

The secrets of this equation can be unlocked by dividing both sides by the product $X(x)\,T(t)$. This gives

We assume that $X(x)$ and $T(t)$ are non-zero (except possibly at isolated points).

$$\frac{1}{X}\frac{d^2X}{dx^2} = \frac{1}{c^2}\frac{1}{T}\frac{d^2T}{dt^2}.$$

Now, this equation has a very interesting property. Because the function $T(t)$ does not appear on the left-hand side, the expression to the left of the equals sign is a function of x only, and does not depend on t. Similarly, the right-hand side is a function of t only, and does not depend on x. But since these expressions are equal, neither expression can depend on either x or t. That means that both sides of the equation are equal to the *same* constant, which we call μ. We can therefore write

$$\frac{1}{X}\frac{d^2X}{dx^2} = \mu = \frac{1}{c^2}\frac{1}{T}\frac{d^2T}{dt^2}.$$

So equation (11) has yielded two ordinary differential equations:

$$\frac{1}{X}\frac{d^2X}{dx^2} = \mu \quad \text{and} \quad \frac{1}{c^2}\frac{1}{T}\frac{d^2T}{dt^2} = \mu.$$

Multiplying the first equation by $X(x)$ and the second by $T(t)$ gives

$$\frac{d^2X}{dx^2} = \mu X \tag{12}$$

and

$$\frac{d^2T}{dt^2} = c^2\mu\, T. \tag{13}$$

These ordinary differential equations for $X(x)$ and $T(t)$ must be satisfied in order for the product function $X(x)\,T(t)$ to be a solution of the wave equation (8). Conversely, the wave equation is satisfied by $X(x)\,T(t)$ if $X(x)$ satisfies equation (12) and $T(t)$ satisfies equation (13). The constant μ is called the **separation constant**. We have no information about this constant at this stage, but we can say that the same constant appears in both equation (12) and equation (13).

The ordinary differential equations (12) and (13) are linear and homogeneous, and they can both be solved using the methods of Unit 3. The nature of the solutions depends on the value of the separation constant μ, and we will consider three cases in turn, depending on whether μ is positive, negative or equal to zero. In each case we will determine the form of the solutions of equations (12) and (13), and consider whether these solutions can satisfy the given boundary conditions.

Separation constant positive

If $\mu > 0$, we can write $\mu = k^2$, where k is a real positive constant. Then equation (12) can be solved by substituting in the trial solution $X(x) = \exp(\lambda x)$. This leads to the auxiliary equation $\lambda^2 = \mu = k^2$, so $\lambda = \pm k$ and the general solution is

$$X(x) = A\exp(kx) + B\exp(-kx), \tag{14}$$

where A and B are arbitrary constants.

We could easily determine the solution for $T(t)$ using the same approach. We will not do this because the form of $T(t)$ is irrelevant for our purposes. We need to know only that the product function takes the form $X(x)\,T(t)$, where $X(x)$ is given by equation (14).

Having determined the form of the solution, we now consider whether the boundary conditions can be satisfied. The displacement $u(x,t) = X(x)\,T(t)$ must be zero at both ends of the string ($x = 0$ and $x = L$) for all positive values of t. This implies that the function $X(x)$ must satisfy the boundary conditions

$$X(0) = X(L) = 0. \tag{15}$$

We consider the conditions $X(0) = 0$ and $X(L) = 0$ in turn. For the function $X(x)$ in equation (14), the condition $X(0) = 0$ gives

$$A + B = 0,$$

and the condition $X(L) = 0$ gives

$$A\exp(kL) + B\exp(-kL) = 0.$$

Combining these equations gives

$$A\big(\exp(kL) - \exp(-kL)\big) = 0.$$

Since both k and L are positive, $kL > 0$, and the only way of satisfying this equation is to take $A = 0$. This gives $u(x,t) = 0$, which does solve the partial differential equation, but in a very dull way. It corresponds to a string that remains permanently in its equilibrium state, not vibrating at all. Such a solution is often referred to as a **trivial solution**, and is not the solution we are seeking.

For $kL > 0$, $\exp(kL) > 1$ and $\exp(-kL) < 1$.

Separation constant negative

If $\mu < 0$, we can write $\mu = -k^2$, where k is a real positive constant. Then equations (12) and (13) become

$$\frac{d^2X}{dx^2} = -k^2X, \tag{16}$$

$$\frac{d^2T}{dt^2} = -k^2c^2T. \tag{17}$$

Again, we concentrate on the first of these equations. This can be recognised as the 'equation of simple harmonic motion' discussed in Unit 3, and it has the general solution

$$X(x) = C\cos(kx) + D\sin(kx), \tag{18}$$

where C and D are arbitrary constants. Let us see whether this function can satisfy the given boundary conditions (15). Applying the condition $X(0) = 0$ to the function in equation (18) gives $C = 0$, so the solution becomes

$$X(x) = D\sin(kx).$$

The condition $X(L) = 0$ then requires that either $D = 0$ or $\sin(kL) = 0$. The first possibility corresponds to the trivial solution $u(x,t) = 0$ mentioned earlier. The second possibility is more interesting. It is satisfied if, and only if, k takes one of the special set of values

$$k = \frac{n\pi}{L}, \quad \text{where } n \text{ is an integer,}$$

and this gives a set of solutions

$$X(x) = D\sin\left(\frac{n\pi x}{L}\right).$$

In fact, the values of n can be restricted further. The value $n = 0$ can be omitted because it gives the trivial solution $u(x,t) = 0$. Also, all negative values of n can be omitted because changing the sign of n is equivalent to changing the sign of D, which is an arbitrary constant anyway. We can therefore say that the most general solution of equation (16), consistent with the boundary conditions, is

$$X(x) = D\sin\left(\frac{n\pi x}{L}\right), \quad \text{where } n = 1, 2, 3, \ldots.$$

We will return to consider the corresponding solution for $T(t)$ shortly.

Separation constant equal to zero

If $\mu = 0$, the equation for $X(x)$ is

$$\frac{d^2X}{dx^2} = 0.$$

The solution of this equation is

$$X(x) = Fx + G,$$

where F and G are arbitrary constants. The boundary condition $X(0) = 0$ gives $G = 0$, so the solution becomes $X(x) = Fx$. The boundary condition $X(L) = 0$ then gives $F = 0$. So $F = G = 0$, and the only solution consistent with the boundary conditions is the trivial solution $u(x,t) = 0$.

Review

Let us review what has been done. We looked for special solutions of the wave equation that are *product functions* of the form $X(x)\,T(t)$. We then saw that the functions $X(x)$ and $T(t)$ must obey the ordinary differential equations (12) and (13), which both involve the same separation constant μ.

We then considered whether the solutions of equation (12) can satisfy the boundary conditions (15). Assuming that μ is a positive constant, or zero, gave functions that do not obey the boundary conditions, or are trivial and of no interest. However, trying a negative value of the separation constant (writing $\mu = -k^2$, where k is a positive constant) gave a set of non-trivial solutions that do obey the boundary conditions. Whenever you try a solution by separation of variables, you need to check what happens for both signs of the separation constant (and you usually need to consider $\mu = 0$ separately as well); you cannot anticipate which choices will give useful solutions.

In order for the wave equation, with its associated boundary conditions, to have a non-trivial product solution $X(x)\,T(t)$, the separation constant μ must be negative. The allowed negative values of μ are not arbitrary.

Writing $\mu = -k^2$, where k is a real positive constant, we have seen that the allowed values of k are

$$k_n = \frac{n\pi}{L} \quad \text{for } n = 1, 2, 3, \ldots,$$

so the allowed values of the separation constant μ are

$$\mu_n = -k_n^2 = -\frac{n^2\pi^2}{L^2}. \tag{19}$$

Corresponding to each of these values, there is a solution for $X(x)$:

$$X_n(x) = D\sin\left(\frac{n\pi x}{L}\right). \tag{20}$$

We now consider the functions $T(t)$. The *same* separation constant occurs in the differential equations for $X(x)$ and $T(t)$, so if we are looking for the function $T(t)$ that accompanies the solution $X_n(x)$ in equation (20), we must use the value $\mu_n = -k_n^2$ in the differential equation for $T(t)$. Hence equation (17) takes the form

$$\frac{d^2T_n}{dt^2} = -k_n^2c^2T_n.$$

This has general solution

$$\begin{aligned} T_n(t) &= \alpha\cos(k_nct) + \beta\sin(k_nct) \\ &= \alpha\cos\left(\frac{n\pi ct}{L}\right) + \beta\sin\left(\frac{n\pi ct}{L}\right), \end{aligned} \tag{21}$$

where α and β are arbitrary constants.

To obtain the possible product functions $u_n(x,t) = X_n(x)\,T_n(t)$, it only remains to multiply together the expressions in equations (20) and (21). We combine the constants by writing $A_n = \alpha D$ and $B_n = \beta D$. The resulting solution is then

$$u_n(x,t) = \sin\left(\frac{n\pi x}{L}\right)\left[A_n\cos\left(\frac{n\pi ct}{L}\right) + B_n\sin\left(\frac{n\pi ct}{L}\right)\right], \tag{22}$$

where A_n and B_n are arbitrary constants and $n = 1, 2, 3, \ldots$.

Equation (22) gives a whole family of solutions, each member of which satisfies the wave equation (8) and its boundary conditions (9). The arbitrary constants A_n and B_n need not be the same for different members of this family, so it is appropriate that they are labelled by the subscript n.

The function in equation (7) is a member of this family with $n = 1$, $A_1 = 1$ and $B_1 = 0$.

The initial displacement of the string for the product solution $u_n(x,t)$ is found by substituting $t = 0$ in equation (22). This gives

$$u_n(x,0) = A_n\sin\left(\frac{n\pi x}{L}\right). \tag{23}$$

The initial displacements for the first three solutions in family (22) are shown in Figure 7 (taking $A_n = 1$). These are the initial shapes of the string. Of course, these shapes are rather special, and do not correspond to the actions of any guitar player!

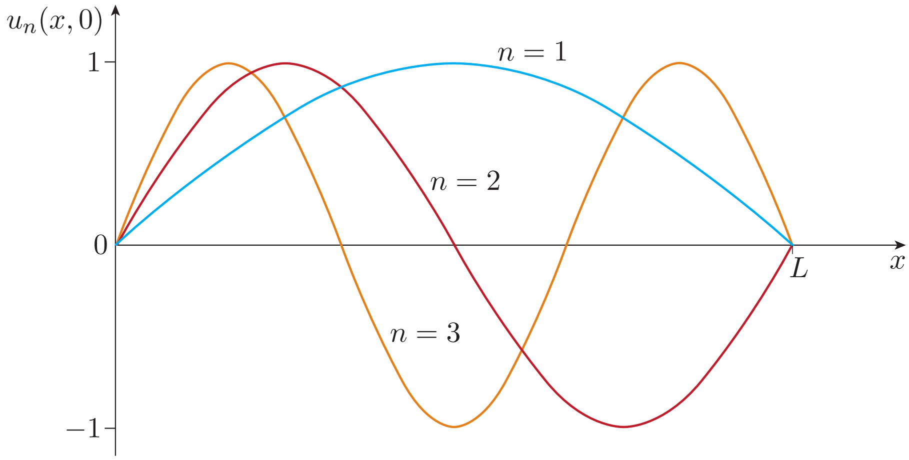


Figure 7 Initial displacements at $t = 0$ for the first three solutions in the family (22), taking $A_1 = A_2 = A_3 = 1$

Once the string is released, its motion obeys equation (22). The term in square brackets scales the shape described by $\sin(n\pi x/L)$ by a factor that oscillates sinusoidally in time. The motion is that of a *standing wave* – a wave that oscillates without travelling through space. For example, if $\sin(n\pi x/L) = 0$ at a particular point, then the disturbance will always be equal to zero at that point; this corresponds to the fact that the nodes of the standing wave remain fixed in space. Each solution in the family (22) has a definite angular frequency $\omega_n = n\pi c/L$. As n increases, ω_n increases, corresponding to a higher frequency of oscillation of the string.

Eigenvalues and eigenfunctions

In looking for solutions of the wave equation in the form $X(x)\,T(t)$, we were led to consider the ordinary differential equation

$$\frac{d^2X}{dx^2} = \mu X, \qquad \text{(Eq. 12)}$$

with boundary conditions $X(0) = X(L) = 0$. It is a remarkable fact that this equation has acceptable solutions (satisfying the boundary conditions) only for certain values of μ, namely

$$\mu_n = -\frac{n^2\pi^2}{L^2}, \quad n = 1, 2, 3, \ldots.$$

Corresponding to each of these allowed values, there is a solution

$$X_n(x) = \sin\left(\frac{n\pi x}{L}\right), \quad n = 1, 2, 3, \ldots.$$

The special values μ_n that allow a solution are called **eigenvalues**, and the corresponding solutions $X_n(x)$ are called **eigenfunctions**.

Also, the functions $T_n(t)$ in equation (21) are eigenfunctions of differential equation (13).

When each solution $X_n(x)$ is joined to its partner $T_n(t)$, we get a solution to the wave equation with a sinusoidal time dependence characterised by a definite angular frequency $\omega_n = n\pi c/L$.

Matrices, normal modes and quantum mechanics

There are strong analogies with concepts met earlier in the module, and important applications to science and engineering.

- Recall that a matrix equation of the form

  $$\mathbf{A}\mathbf{x} = \lambda\mathbf{x},$$

  where $\mathbf{A}$ is a given square matrix, $\mathbf{x}$ is a column matrix, and λ is a number, is called an *eigenvalue equation*. The values of λ that allow solutions to be found for $\mathbf{x}$ are called *eigenvalues*, and the corresponding solutions $\mathbf{x}$ are called *eigenvectors*. Equation (12) is analogous to this, but instead of a matrix $\mathbf{A}$ acting on a vector $\mathbf{x}$, we have a differential operator d^2/dx^2 (supplemented by boundary conditions) acting on a function $X(x)$.
- Unit 6 discussed the oscillations of systems of particles, such as the atoms in a carbon dioxide molecule. You saw that there are some characteristic patterns of displacement that oscillate with definite angular frequencies. These patterns are called *normal modes*. They exist only at a discrete set of angular frequencies, which are determined by finding the eigenvalues of a matrix. The standing waves on a string are so reminiscent of this that they too are referred to as **normal modes**.
- In quantum mechanics, there is a partial differential equation called the *Schrödinger equation*. This is not the same as the wave equation for a string, but there are similarities. The Schrödinger equation can be solved for a hydrogen atom, using the method of separation of variables, much as we have done here. Again, there are eigenvalues and eigenfunctions: these are interpreted, respectively, as the allowed energies and the corresponding states of the atom. Because the eigenvalues form a discrete set, the atom has a discrete set of allowed energies. This is known as the *quantisation of energy*.

Exercise 5

Apply the method of separation of variables to the partial differential equation

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^4 u}{\partial x^4},$$

which occurs in the theory of bending elastic rods. Write $u(x,t) = X(x)\,T(t)$, and establish ordinary differential equations for the functions $X(x)$ and $T(t)$. Do not attempt to solve these equations.

Exercise 6

Apply the method of separation of variables to the partial differential equation

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}(xu) + \frac{\partial^2 u}{\partial x^2},$$

which occurs in the theory of diffusion of solid particles in a fluid. Write $u(x,t) = X(x)\,T(t)$, and establish ordinary differential equations for the functions $X(x)$ and $T(t)$. Do not attempt to solve these equations.

1.3 Superposition and the general solution

So far, we have found a family of solutions of the wave equation (8) that satisfy the boundary conditions (9). These solutions, specified in equation (22), are all of the product form $X(x)\,T(t)$. You might ask why we decided to look for solutions like this. The reason is not very profound – it is just that these solutions are found relatively easily (provided that the method of separation of variables works at all).

However, we cannot pretend that every solution is a product solution. For example, equation (23) and Figure 7 show that the product solutions are produced by very special initial conditions at $t = 0$. When a guitar string is plucked at its midpoint, as in Figure 5, the initial conditions are quite different, and the subsequent motion of the string cannot be described by a product solution.

Fortunately, there is a way ahead. The wave equation is linear, and so are all the partial differential equations in this unit, which means that the principle of superposition applies. In the specific context of linear second-order partial differential equations, the **principle of superposition** states that if $u_1(x,t)$ and $u_2(x,t)$ are solutions of the equation, then any function of the form

$$u(x,t) = a_1\,u_1(x,t) + a_2\,u_2(x,t), \tag{24}$$

where a_1 and a_2 are constants, is also a solution of the equation.

The following exercise asks you to verify that this principle applies to the wave equation, and to show how it applies in the presence of the usual boundary conditions.

Exercise 7

Suppose that the functions $u_1(x,t)$ and $u_2(x,t)$ satisfy the wave equation

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{c^2}\,\frac{\partial^2 u}{\partial t^2},$$

together with the boundary conditions for fixed ends

$$u(0,t) = u(L,t) = 0.$$

Show that the linear combination $u = a_1u_1 + a_2u_2$, where a_1 and a_2 are any constants, is a solution of the same partial differential equation and satisfies the same boundary conditions.

The principle of superposition takes two solutions and generates a third. Repeating this process, we can add further solutions and expand the linear combination without limit, generating many more solutions. Moreover, if all the individual solutions satisfy the boundary conditions $u(0,t) = 0$ and $u(L,t) = 0$, then so does the linear combination formed from them.

Starting from the product solutions in equation (22), it follows that *any* linear combination of the form

$$u(x,t) = \sum_{n=1}^{\infty} \sin\left(\frac{n\pi x}{L}\right) \left[A_n \cos\left(\frac{n\pi ct}{L}\right) + B_n \sin\left(\frac{n\pi ct}{L}\right)\right], \qquad (25)$$

where A_n and B_n are constants, is a solution of the wave equation that satisfies the boundary conditions for fixed ends, $u(0,t) = 0$ and $u(L,t) = 0$.

The sum in equation (25) may stop after a finite number of terms; this happens if all the A_n and B_n are equal to zero beyond a certain value of n. However, it is also possible that the sum continues without ever ending. The value of such an infinite sum is defined as the limiting value of the sum of the first N terms, as N tends to infinity. However, this technicality is really beyond the scope of this unit. We assume that sums of this type are 'well-behaved' so that there is no difficulty, for example, in differentiating $u(x,t)$ by differentiating each term in the infinite series.

The principle of superposition greatly extends the range of known solutions. In fact, it delivers something even more powerful. It turns out that for a string that is anchored at $x = 0$ and $x = L$, *every* solution can be written in the form (25). In other words, equation (25) is the **general solution** of the wave equation subject to these conditions.

General solution for motion of a string

The general solution of the wave equation on the interval from 0 to L with boundary conditions $u(0,t) = u(L,t) = 0$ is

$$u(x,t) = \sum_{n=1}^{\infty} \sin\left(\frac{n\pi x}{L}\right) \left[A_n \cos\left(\frac{n\pi ct}{L}\right) + B_n \sin\left(\frac{n\pi ct}{L}\right)\right], \qquad (26)$$

where A_n and B_n are arbitrary constants.

This is a wonderful gift. We started with a restricted family of solutions – the product solutions. These are just a small subset of all the possible solutions, but it turns out that *any* solution can be expressed as a linear combination of them. We do not prove this fact, but we can say that it is a common feature of many linear partial differential equations.

For different partial differential equations, the functions that emerge from the method of separation of variables are not always sines and cosines, but they often provide a set of functions that is broad enough for any solution to be expressed as a linear combination of them. Such a family of functions is sometimes said to form a **complete set** for the problem at hand.

1.4 Initial conditions and Fourier series

The constants $A_1, A_2, A_3, \ldots$ and $B_1, B_2, B_3, \ldots$ in the general solution are determined by the initial conditions.

An important case is that of a plucked string, released from rest at $t = 0$, with an initial displacement specified by a function $f(x)$. These initial conditions are described by the equations

$$\frac{\partial u}{\partial t}(x,0) = 0, \quad u(x,0) = f(x), \quad 0 \le x \le L. \tag{27}$$

Consider the first condition, which describes release from rest. Differentiating both sides of equation (26) with respect to t, and assuming that the derivative of the right-hand side is obtained by differentiating each term in the sum, we get

$$\frac{\partial u}{\partial t} = \sum_{n=1}^{\infty} \sin\left(\frac{n\pi x}{L}\right)\left(\frac{n\pi c}{L}\right)\left[-A_n \sin\left(\frac{n\pi ct}{L}\right) + B_n \cos\left(\frac{n\pi ct}{L}\right)\right].$$

Setting $\partial u/\partial t = 0$ at $t = 0$ then gives

$$0 = \sum_{n=1}^{\infty}\left(\frac{n\pi c}{L}\right) B_n \sin\left(\frac{n\pi x}{L}\right). \tag{28}$$

One way of satisfying this equation is to take $B_n = 0$ for all n. In fact, the right-hand side of equation (28) is a Fourier series with Fourier coefficients $n\pi c B_n/L$. These Fourier coefficients are uniquely defined by the zero function on the left-hand side, and are all equal to zero, so the *only* way of satisfying equation (28) is to take $B_n = 0$ for all n. The general solution given in equation (26) then reduces to the following expression.

The general solution for a plucked string released from rest is

$$u(x,t) = \sum_{n=1}^{\infty} A_n \sin\left(\frac{n\pi x}{L}\right)\cos\left(\frac{n\pi ct}{L}\right). \tag{29}$$

We must now choose the constants A_n so that the other initial condition is satisfied, namely $u(x,0) = f(x)$, where $f(x)$ describes the displacement of the string at time $t = 0$.

Putting $t = 0$ in equation (29), and using $u(x,0) = f(x)$, we get

$$f(x) = \sum_{n=1}^{\infty} A_n \sin\left(\frac{n\pi x}{L}\right) \quad (0 \le x \le L). \tag{30}$$

The sum on the right-hand side is a Fourier series for the function $f(x)$ that involves sine terms only. At first sight this may seem rather strange because $f(x)$ is not a periodic function, but is defined only over the finite interval $0 \leq x \leq L$. However, you saw in Unit 11 that a function defined over a finite interval can be extended outside this interval to give a periodic function.

Because equation (30) involves sine terms only, we need the *odd periodic extension* here. Note that this choice is determined by the form of equation (30). There is no essential connection between the names used for the coefficients in this equation and the traditional names A_0, A_n and B_n used in the Fourier series of Unit 11.

To take a definite case, suppose that the string is released from rest by being plucked at its midpoint, which has an initial displacement d. You saw in Example 1 that this initial displacement is described by the piecewise function

$$f(x) = \begin{cases} \dfrac{2d}{L}x & \text{for } 0 \leq x \leq \tfrac{1}{2}L, \\ \dfrac{2d}{L}(L-x) & \text{for } \tfrac{1}{2}L < x \leq L, \end{cases} \tag{31}$$

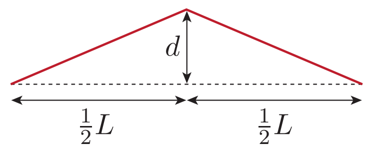


Figure 8 String plucked at its midpoint

and a diagram of this initial displacement is reproduced in Figure 8.

We can extend $f(x)$ to give the periodic function $f_{\text{odd}}(x)$ shown in Figure 9, which is given by the formula

$$f_{\text{odd}}(x) = \begin{cases} f(x) & \text{for } 0 \leq x \leq L, \\ -f(x) & \text{for } -L < x < 0, \end{cases}$$

$$f_{\text{odd}}(x + 2L) = f_{\text{odd}}(x).$$

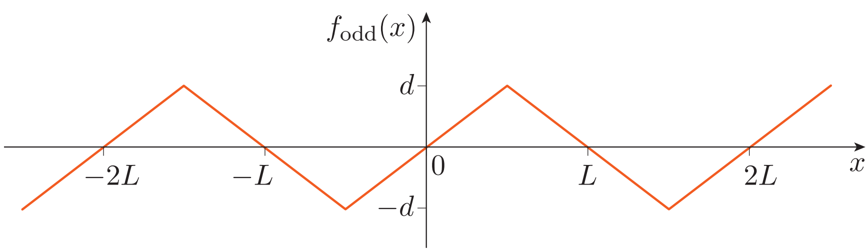


Figure 9 The odd periodic extension of the function in Figure 8

This is the odd periodic extension of $f(x)$, and it has fundamental period $2L$. Because the functions $f(x)$ and $f_{\text{odd}}(x)$ are identical in the region of interest $0 \leq x \leq L$, the constants A_n required in equation (30) are identical to the Fourier coefficients of $f_{\text{odd}}(x)$. Since $f_{\text{odd}}(x)$ is an odd function with period $2L$, we have

$$A_n = \frac{4}{2L}\int_0^L f_{\text{odd}}(x)\sin\left(\frac{n\pi x}{L}\right)dx.$$

See Unit 11, equation (37) with suitably adjusted notation.

Finally, the functions $f(x)$ and $f_{\text{odd}}(x)$ are identical throughout the interval $0 \leq x \leq L$, so we have the following result.

$$A_n = \frac{2}{L}\int_0^L f(x)\sin\left(\frac{n\pi x}{L}\right)dx, \quad n = 1, 2, 3, \ldots. \tag{32}$$

To illustrate the use of a periodic extension, we have looked at the function illustrated in Figures 8 and 9, but it is clear that the same argument would work for any initial displacement. Hence equation (32) gives a general formula for the coefficients A_n in equations (29) and (30) – we just have to insert the function $f(x)$ that describes the initial displacement of the plucked string, as it is released from rest.

For the initial displacement in equation (31) and Figure 8, the Fourier coefficients are

$$A_n = \frac{4d}{L^2}\left[\int_0^{L/2} x\sin\left(\frac{n\pi x}{L}\right)dx + \int_{L/2}^{L}(L-x)\sin\left(\frac{n\pi x}{L}\right)dx\right].$$

As is often the way, the Fourier integrals are messy to evaluate. There is nothing really difficult, but patience and care are essential. Fortunately, we have already calculated these integrals in Example 11 of Unit 11, so we can just quote the result. In this case, the Fourier coefficients are given by

$$A_n = \frac{8d}{n^2\pi^2}\sin\left(\frac{n\pi}{2}\right),$$

so the values of the first few coefficients are

$$A_1 = \frac{8d}{\pi^2}, \quad A_2 = 0, \quad A_3 = -\frac{8d}{9\pi^2}, \quad A_4 = 0, \quad A_5 = \frac{8d}{25\pi^2}.$$

Substituting these coefficients into equation (29), we conclude that the displacement of the plucked string at any time $t > 0$ is

$$\begin{aligned} u(x,t) = \frac{8d}{\pi^2}\Bigg[&\sin\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi ct}{L}\right) - \frac{1}{9}\sin\left(\frac{3\pi x}{L}\right)\cos\left(\frac{3\pi ct}{L}\right) \\ &+ \frac{1}{25}\sin\left(\frac{5\pi x}{L}\right)\cos\left(\frac{5\pi ct}{L}\right) - \cdots\Bigg]. \end{aligned} \tag{33}$$

The exact solution is given by an infinite sum of terms, but a very good approximation is obtained by adding the first 30 terms on a computer. When this is done, the shape of the string is predicted to vary as shown in Figure 10. You may find this prediction surprising, especially the kinks that exist throughout the motion of the string. But if one films the motion of a real string that is released in the way assumed, the film captures a succession of images that match Figure 10 almost exactly!

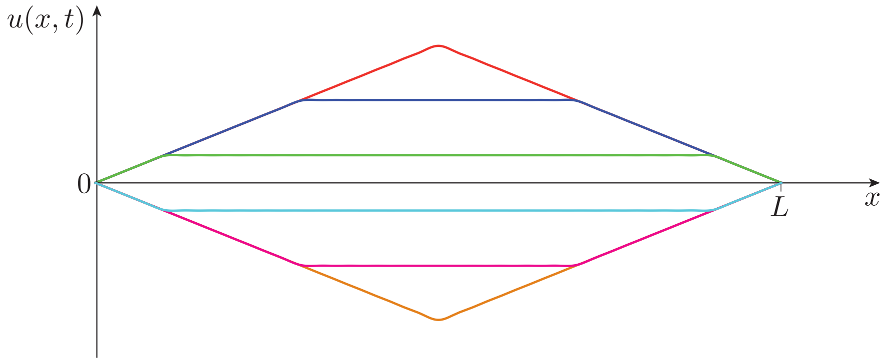


Figure 10 The motion predicted by equation (33), with the time sequence red, dark blue, green, cyan, magenta, orange, magenta, etc.; this shows the displacements at a sequence of times

Fourier's masterpiece

Fourier series were invented to aid the solution of partial differential equations by separation of variables.

Joseph Fourier (1768–1830) is best remembered for the contributions in his work *The Analytic Theory of Heat*, published in 1822, which combined the results of two decades of investigation. This work developed most of the ideas contained in Unit 11 as well as this unit. Fourier derived the heat equation (2) and solved it using the method of separation of variables. He represented the initial condition as a series in the form (30), now known as a Fourier series, and discovered the technique to determine the coefficients A_n.

Alternative initial conditions

The general solution in equation (26) can be adapted to deal with the case where the initial conditions are

$$u(x,0) = 0, \quad \frac{\partial u}{\partial t}(x,0) = v(x), \quad 0 \le x \le L, \tag{34}$$

that is, where the initial displacement of the string is zero, but the initial velocity is given by a function $v(x)$. This corresponds more closely to a piano string that is struck by one of the piano's hammers than to a guitar string that is plucked and released from rest.

Because the coefficients A_n in equation (26) are Fourier coefficients of the initial displacement, which is equal to zero for all x, we must have $A_n = 0$ for all $n = 1, 2, \ldots$. The general solution for the motion of the string can then be written in the form

$$u(x,t) = \sum_{n=1}^{\infty} B_n \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{n\pi ct}{L}\right). \tag{35}$$

The coefficients B_n can be determined by an approach similar to that used for the initially stationary string, as the following exercise shows.

Exercise 8

Consider a string, clamped at $x = 0$ and at $x = L$, with a displacement $u(x,t)$ that satisfies the wave equation, with boundary conditions $u(0,t) = u(L,t) = 0$ for $t \geq 0$.

At $t = 0$, the displacement is zero, so $u(x,0) = 0$. However, the string is set in motion so that its initial velocity at x is $v(x)$, where $v(x)$ is a specified function. The odd periodic extension of $v(x)$ has Fourier coefficients C_n, so for $0 \leq x \leq L$ the initial velocity of the string is given by

$$v(x) = \sum_{n=1}^{\infty} C_n \sin\left(\frac{n\pi x}{L}\right).$$

Use equation (35) to express the coefficients B_n in terms of the Fourier coefficients C_n.

The methods used in this section can be applied to a variety of linear homogeneous partial differential equations, not just the wave equation. The general method is summarised in the following procedure, which can be used for all the partial differential methods in this unit.

Procedure 1 The method of separation of variables

Given a linear homogeneous partial differential equation with dependent variable u and independent variables x and t, subject to given boundary and initial conditions, a solution can often be found by the following steps.

1. Write the unknown function $u(x,t)$ as a product of functions of one variable:

   $$u(x,t) = X(x)\,T(t).$$

   Find the required partial derivatives of u in terms of the ordinary derivatives of the functions X and T.
2. Substitute the partial derivatives found in Step 1 into the partial differential equation. Rearrange the equation so that each side consists of a function of a single independent variable. Equate each side of the rearranged equation to the same separation constant μ, and hence obtain ordinary differential equations for X and T.
3. Use the given boundary conditions for u to find boundary conditions for X.

4. Solve the differential equation for X, and apply the boundary conditions. Consider different choices for the separation constant μ. (Typically, the solutions $X(x)$ take a different form depending on whether the separation constant is positive, negative or zero.) The boundary conditions generally produce a discrete set of solutions $X_n(x)$ and a corresponding discrete set of values μ_n for the separation constant.
5. For each allowed μ_n, determine the corresponding solution $T_n(t)$ of the differential equation for $T(t)$.
6. Combine $X_n(x)$ and $T_n(t)$ to obtain a family of product solutions

$$u_n(x,t) = X_n(x)\,T_n(t), \quad n = 1, 2, 3, \ldots.$$

Express the general solution as an infinite linear combination of these product solutions containing a set of coefficients. For example,

$$u(x,t) = \sum_{n=1}^{\infty} a_n\, u_n(x,t).$$

7. Use the initial conditions and results about Fourier series to determine (when possible) the set of coefficients.

Exercise 9

Use Steps 1–6 of Procedure 1 to find the general solution of the partial differential equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial t^2} = 0,$$

subject to boundary conditions

$$u(0,t) = u(1,t) = 0, \quad t \geq 0.$$

This equation is known as the two-dimensional *Laplace equation*.

2 The diffusion equation

The **diffusion equation** takes the form

$$\frac{\partial c}{\partial t} = D\,\frac{\partial^2 c}{\partial x^2}, \tag{36}$$

where D is a positive constant called the **diffusion coefficient**, and $c = c(x,t)$ is a function of x and t. In solving this equation, the aim is to find a function $c(x,t)$ that satisfies the equation, subject to given boundary and initial conditions. The diffusion equation is one of the most widely studied partial differential equations, and it arises in many different contexts.

The section begins by discussing the physical concepts that lie behind the diffusion equation before going on to derive it. *This material will not be assessed or examined.* Nevertheless, the process of deriving a partial differential equation from physical assumptions is a vital skill for scientists and applied mathematicians, and you should study Subsections 2.1–2.4 to see an example of this process in action.

Subsection 2.5 uses the method of separation of variables to solve the diffusion equation for a particular example; this skill is assessable.

2.1 Diffusion

On a microscopic scale, matter consists of molecules, with each chemical substance having its own type of molecule. Very often, samples of matter are mixtures of different types of molecule. For example, air contains a mixture of nitrogen and oxygen molecules, with small quantities of many other molecules.

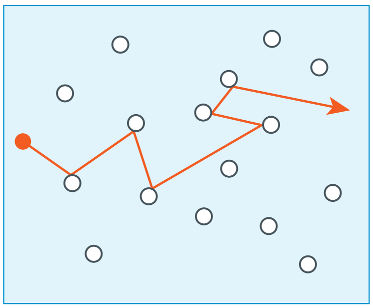


Figure 11 A carbon dioxide molecule (coloured) moves erratically as it collides with other molecules in air

The molecules are always in motion, and in gases or liquids these motions are random and unpredictable. The molecules are very small, typically about 10^{-9} m across, and at room temperature they move very quickly (at speeds of about $300\,\mathrm{m\,s^{-1}}$). They travel only very short distances in between collisions: in a gas they move about 10^{-7} m before colliding and changing direction. Figure 11 is a schematic illustration of the motion of a carbon dioxide molecule in air.

This random motion of molecules gives rise to an important mechanism for mixing substances: it results in substances spreading out in space, as illustrated in Figure 12. This process, called **diffusion**, mixes substances by means of the microscopic random motion of molecules, without the need for any macroscopic motion (such as the stirring motion that helps to dissolve sugar in coffee).

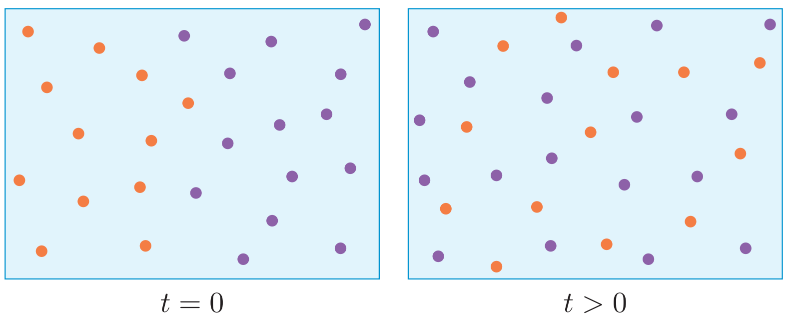


Figure 12 The random motion of molecules leads to mixing of substances

The process of diffusion is vitally important for biological processes. For example, your body creates carbon dioxide as a waste product, and this must be removed from your tissues very efficiently. Your blood vessels and lungs play an important role in carrying carbon dioxide out of your body, but it is diffusion that enables carbon dioxide molecules to move out of your cells and into the blood vessels.

2.2 Concentration and flux density

In principle, diffusion can be described by tracking the motion of a vast number of molecules, but this is obviously impractical. For most purposes, we do not care about the motion of individual molecules, but we want to know how the molecules as a whole reposition themselves. In this subsection, we introduce two quantities – *concentration* and *flux density* – that help us to model the process of diffusion.

Diffusion generally refers to molecules of a definite type or species, mixed in with other molecules that are not of interest.

Molecular concentration

The **concentration** of molecules of a given type at position $\mathbf{r}$ is the number of those molecules per unit volume, found in a small region centred on $\mathbf{r}$.

If the region has volume ΔV and contains ΔN molecules of the given type at time t, then the concentration is

$$c(\mathbf{r}, t) = \frac{\Delta N}{\Delta V}. \tag{37}$$

Figure 13 illustrates this definition for a two-dimensional case.

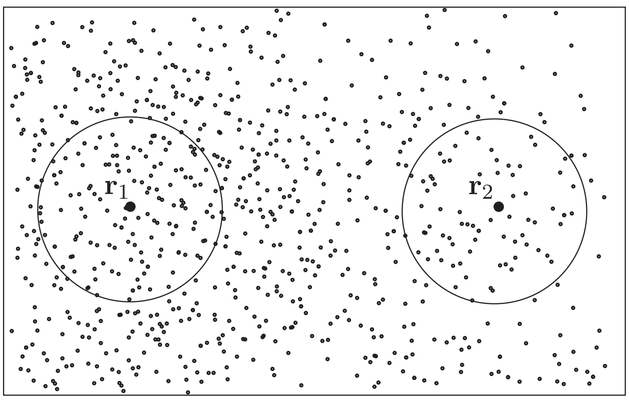


Figure 13 The distribution of molecules of a particular type in two dimensions (other molecules are not shown). The circles define imaginary regions centred on $\mathbf{r}_1$ and $\mathbf{r}_2$. Counting molecules of the given type in these regions shows that their concentration is higher at $\mathbf{r}_1$ than at $\mathbf{r}_2$.

To give a detailed description of the distribution of molecules, the volume ΔV should be small on an everyday scale. But it must not be too small, or it is unlikely to contain any molecules of the given type! In practice, a suitable compromise can generally be reached, giving a function $c(\mathbf{r}, t)$ that varies smoothly with $\mathbf{r}$ and t.

We also need to describe the motion of molecules. In the case of diffusion, the molecules are moving around at random, but we can talk about the net motion in a given direction.

Suppose that we wish to describe the net flow of molecules of the given type *in the x-direction* at a particular position $\mathbf{r}$. Then we imagine a small *imaginary* planar surface element that is centred on position $\mathbf{r}$. The surface element has area ΔA, and it is oriented so that it is perpendicular to the x-direction, with its unit normal vector pointing in the x-direction (see Figure 14).

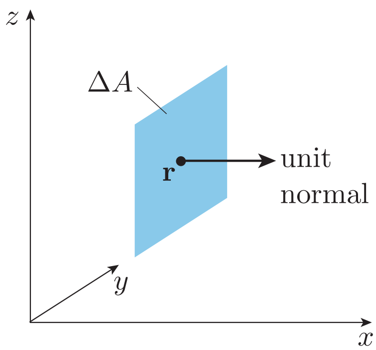


Figure 14 An imaginary surface element used to define flux density

In the small time interval between t and $t + \delta t$, we count the number of molecules of the given type that pass through this surface element in the sense of increasing x (i.e. from the back to the front of the surface in Figure 14). Let this number be δn^+. We also count the corresponding number of molecules passing through the surface in the opposite sense. Let this number be δn^-. We care only about the *net migration* across the surface in the x-direction, which is defined by

$$\delta n = \delta n^+ - \delta n^-.$$

We expect δn to be proportional to the time interval δt, and to the area ΔA. We therefore write

$$\delta n = J_x \, \Delta A \, \delta t, \tag{38}$$

where J_x is a quantity called the *flux density* in the x-direction. Making J_x the subject of this equation leads to the following definition.

Molecular flux density

For a given type of molecule, the **flux density** in the x-direction at position $\mathbf{r}$ and time t is defined as

$$J_x(\mathbf{r}, t) = \frac{1}{\Delta A} \frac{\delta n}{\delta t}, \tag{39}$$

where ΔA is the area of a surface element, centred on $\mathbf{r}$ and perpendicular to the x-axis, and $\delta n/\delta t$ is the rate of net migration across this surface in the direction of increasing x at time t.

The same sort of caveats surround this definition as for concentration: the area ΔA and the time interval δt should be taken to be small, but not too small! Again, this is no cause for concern, and the flux density defined by equation (39) can be assumed to vary smoothly in space and time.

A comment on notation

Note that δn in the above equations is the number of molecules migrating across a surface in time δt. It should not be confused with ΔN in equation (37), which is the number of molecules in a small volume.

In this section, we use Δ to indicate small quantities associated with a small volume or a small area, and δ to indicate small quantities associated with a small time interval.

2.3 The equation of continuity and Fick's law

Our aim is to derive the diffusion equation (36), which is a partial differential equation for the concentration c of molecules of a particular type. To achieve this, we use two different relationships between the concentration c and the flux density J_x. Then, by eliminating the flux density from these equations, we obtain the diffusion equation.

This subsection develops the two required relationships, beginning with the equation of continuity for diffusing molecules, which is very similar to the equation of continuity for a fluid discussed in Unit 10. Because equation (36) contains only one spatial variable, x, we consider a one-dimensional situation.

The equation of continuity

Consider the diffusion of molecules in a narrow glass tube containing a gas. To take a concrete example, suppose that the tube contains air with a small amount of carbon dioxide gas. The tube is aligned with the x-axis, and we focus on the small element of it that lies between x and $x + \Delta x$, where Δx is small. Taking the internal cross-sectional area of the tube to be ΔA, the volume of gas contained in the volume element is $\Delta V = \Delta A\,\Delta x$. If at time t the concentration of carbon dioxide molecules is $c(x,t)$, then the number of carbon dioxide molecules in the element is

$$\Delta N = c(x,t)\,\Delta V = c(x,t)\,\Delta A\,\Delta x. \tag{40}$$

We now make the key assumption that carbon dioxide molecules are neither created nor destroyed in the tube. This implies that no chemical reactions take place in the tube that create carbon dioxide molecules from other substances or that split carbon dioxide molecules apart. Assuming that the walls of the glass tube are impermeable to gases, it follows that any change in ΔN must be caused by molecules that flow into or out of the element by crossing one of the two plane surfaces of area ΔA at its ends. We consider the flows of carbon dioxide molecules through these surfaces in the time interval between t and $t + \delta t$ (see Figure 15).

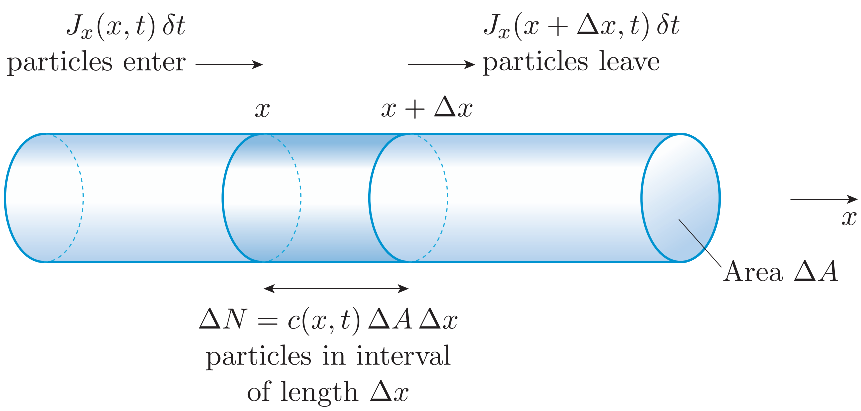


Figure 15 The equation of continuity is derived by considering the change in concentration that results from flow into and out of a volume element

From equation (38), the net number of carbon dioxide molecules that *enter* the volume element by passing through the left-hand surface at x is

$$\delta n(x) = J_x(x,t)\,\Delta A\,\delta t.$$

Similarly, the net number of carbon dioxide molecules that *leave* the volume element by passing through the right-hand surface at $x + \Delta x$ is

$$\begin{aligned}\delta n(x+\Delta x) &= J_x(x+\Delta x, t)\,\Delta A\,\delta t\\ &\simeq \left[J_x(x,t) + \frac{\partial J_x}{\partial x}(x,t)\,\Delta x\right]\Delta A\,\delta t,\end{aligned}$$

where we have used the first-order Taylor polynomial approximation for $J_x(x+\Delta x, t)$ in the last step.

Taking the difference between $\delta n(x)$ and $\delta n(x+\Delta x)$ gives the net *change* in the number of carbon dioxide molecule in the volume element:

$$\delta(\Delta N) = \delta n(x) - \delta n(x+\Delta x) = -\frac{\partial J_x}{\partial x}(x,t)\,\Delta x\,\Delta A\,\delta t.$$

From equation (40), this can also be expressed in terms of a change in concentration in the volume element:

$$\delta(\Delta N) = \delta c(x,t)\,\Delta A\,\Delta x.$$

Comparing these last two equations, we see that

$$\delta c(x,t) = -\frac{\partial J_x}{\partial x}(x,t)\,\delta t.$$

Finally, we divide by δt and take the limit as $\delta t \to 0$ at constant x, so that $\delta c/\delta t$ becomes the partial derivative $\partial c/\partial t$. We obtain the following result.

The equation of continuity for diffusion

$$\frac{\partial c}{\partial t} + \frac{\partial J_x}{\partial x} = 0. \tag{41}$$

This is the first of the equations that links concentration to flux density.

Fick's law

The second equation linking concentration to flux density is called *Fick's law*. We know from observing the process of diffusion that molecules of a given type tend to move from regions of high concentration to regions of low concentration (see, for example, Figure 12). This suggests that the flux density of diffusing particles might be related to the *gradient* of their concentration. In one dimension, a plausible relation between the flux density J_x and the concentration c is as follows.

Fick's law of diffusion

Fick's law of diffusion states that

$$J_x = -D\,\frac{\partial c}{\partial x}, \tag{42}$$

where D is a positive constant called the **diffusion coefficient**. The minus sign indicates that the net flow is from regions of high concentration to regions of low concentration.

When Fick's law was first proposed in 1855 it was an inspired piece of guesswork. While Fick's law can now be derived from a microscopic theory of diffusion, the methods are far beyond the scope of this module. Together with the equation of continuity, Fick's law leads directly to the diffusion equation, as you will see in the next subsection.

2.4 The diffusion equation

Equations (41) and (42) are two partial differential equations that relate the concentration c to the flux density J_x. If we substitute (42) into (41), we obtain an equation that contains c alone:

$$\frac{\partial c}{\partial t} = -\frac{\partial J_x}{\partial x} = -\frac{\partial}{\partial x}\left(-D\,\frac{\partial c}{\partial x}\right)$$

so

$$\frac{\partial c}{\partial t} = D\,\frac{\partial^2 c}{\partial x^2},$$

which is the diffusion equation in one dimension, x. This is the form of the diffusion equation that is used in this unit. However, *for interest only*, the following box indicates how a diffusion equation arises in three dimensions.

The diffusion equation in three dimensions

In order to extend the diffusion equation to three dimensions, we must first define a *flux density vector*. You have seen how J_x is defined in the x-direction. By orienting surface elements perpendicular to the y- and z-axes, we can also define the flux density J_y in the y-direction and the flux density J_z in the z-direction. It can be shown that these three quantities are the components of a vector

$$\mathbf{J} = J_x\,\mathbf{i} + J_y\,\mathbf{j} + J_z\,\mathbf{k},$$

which is called the **flux density vector**. This is a vector field, and in three dimensions the **equation of continuity** takes the form

$$\frac{\partial c}{\partial t} + \boldsymbol{\nabla}\cdot\mathbf{J} = 0. \tag{43}$$

Moreover, in three dimensions **Fick's law** takes the form

$$\mathbf{J} = -D\,\boldsymbol{\nabla} c, \tag{44}$$

where $\boldsymbol{\nabla} c$ is the gradient of the concentration, and D is the diffusion coefficient.

Combining equations (43) and (44), and using the methods of Unit 10, it can be shown that

$$\frac{\partial c}{\partial t} = D\left[\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2}\right],$$

and this is the **three-dimensional diffusion equation**. It is often expressed in terms of the more compact notation

$$\frac{\partial c}{\partial t} = D\,\nabla^2 c,$$

where

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

is called the **Laplacian operator**.

An interesting facet of the diffusion equation (whether in one dimension or more) is that it is a *deterministic* equation that contains no random numbers, but which nevertheless describes the *random* motion of many molecules. Of course, an important element of diffusion is that the molecules in a gas or liquid make many small unpredictable steps. Many other situations involve a large number of random changes, and the diffusion equation has been adapted to describe a vast range of phenomena. One important application relates to finance.

The Black–Scholes equation

The price of a traded commodity or share rises and falls in an unpredictable manner, similar to a coordinate of a molecule in a gas. Thus a diffusion equation might be used to predict how the future value of a portfolio of shares is expected to vary. A particular form of diffusion equation, known as the *Black–Scholes equation*, is widely used by financial institutions to determine the value of contracts that involve commitments to buy or sell on a date in the future.

Trading ‘options’ represents a vast amount of economic activity, and the value of the diffusion-based model for valuing these contracts was recognised by the award of a Nobel prize in economics in 1997.

2.5 Solving the diffusion equation

This subsection returns to the major theme of this unit – the solution of partial differential equations by the method of separation of variables. It presents a problem involving the diffusion equation, broken down into a number of steps. Study it carefully because it differs in several details from the guitar string problem discussed in Section 1.

Example 2

In this question, you are asked to use the method of separation of variables to solve the diffusion equation in the form

$$\frac{\partial^2 c}{\partial x^2} = \frac{1}{D}\frac{\partial c}{\partial t} \quad (0 < x < 1,\ t > 0)$$

for the function $c(x,t)$, where $D > 0$ is a constant. The equation is subject to the boundary conditions

$$\frac{\partial c}{\partial x}(0,t) = \frac{\partial c}{\partial x}(L,t) = 0 \quad (t > 0)$$

and the initial condition

$$c(x,0) = f(x) \quad (0 \le x \le L).$$

Only one initial condition is needed because the diffusion equation is first-order in time. By contrast, the wave equation is second-order in time and needs two initial conditions.

The solution can be found by completing the following steps.

(a) Use the method of separation of variables, with $c(x,t) = X(x)\,T(t)$, and show that the function $X(x)$ satisfies the differential equation

$$X'' - \mu X = 0 \tag{45}$$

for some constant μ. What boundary conditions must X also satisfy?

(b) Show that if $\mu > 0$, then there are no non-trivial solutions of equation (45).

(c) Show that if $\mu = 0$, then there is a non-trivial solution of equation (45). Determine a form of this solution that satisfies the boundary conditions.

(d) Find the non-trivial solutions of equation (45) satisfying the boundary conditions when $\mu < 0$, stating clearly what values μ is allowed to take.

(e) Find and solve the differential equation that T must satisfy.

(f) Use your answers to write down a family of product solutions $c(x,t) = X(x)\,T(t)$ that satisfy the boundary conditions. You may assume that the general solution of the partial differential equation may be expressed as an arbitrary linear combination of members of this family. Write down an expression for the general solution.

(g) Briefly describe how you would use the initial condition $c(x,0) = f(x)$ to determine the particular solution of the partial differential equation.

Solution

(a) Writing $c(x,t) = X(x)\,T(t)$ and substituting into the diffusion equation gives

$$X''(x)\,T(t) = \frac{1}{D}\,X(x)\,T'(t),$$

and dividing through by $X(x)\,T(t)$ gives

$$\frac{X''(x)}{X(x)} = \frac{1}{D}\,\frac{T'(t)}{T(t)}.$$

For brevity, we use primes to denote derivatives: $X' = dX/dx$ and $T' = dT/dt$, and so on.

Because the left-hand side is a function only of x, and the right-hand side is a function only of t, both sides must be equal to the same separation constant μ, so

$$\frac{X''(x)}{X(x)} = \mu = \frac{1}{D}\,\frac{T'(t)}{T(t)}.$$

Thus we obtain two ordinary differential equations:

$$X'' = \mu X, \quad T' = \mu D T.$$

Noting that $\partial c/\partial x = X'(x)\,T(t)$, the boundary conditions imply that

$$X'(0) = X'(L) = 0.$$

(b) If $\mu = k^2 > 0$, where k is a positive constant, then the differential equation for $X(x)$ has the auxiliary equation $\lambda^2 = k^2$, so $\lambda = \pm k$ and the solutions are of the form

$$X(x) = A\exp(kx) + B\exp(-kx),$$

where A and B are arbitrary constants.

Differentiating $X(x)$ gives

$$X'(x) = kA\exp(kx) - kB\exp(-kx),$$

so the boundary conditions $X'(0) = 0$ and $X'(L) = 0$ become, respectively,

$$kA - kB = 0 \quad \text{and} \quad kA\exp(kL) - kB\exp(-kL) = 0.$$

The first condition implies that $A = B$. Substituting this into the second condition, and remembering that $k \neq 0$, we get either $A = 0$ or $\exp(kL) = \exp(-kL)$. The first possibility is not considered further, because it leads to the trivial solution $c(x,t) = 0$. The second possibility gives

$$\exp(2kL) = 1,$$

which cannot be satisfied for $k > 0$ and $L > 0$. We conclude that there is no non-trivial solution for $\mu > 0$.

(c) If $\mu = 0$, then solutions are of the form

$$X(x) = A + Bx,$$

where A and B are arbitrary constants. The derivative of this solution is $X'(x) = B$. This time, both the boundary conditions imply that $B = 0$, but they do not constrain A. Therefore if $\mu = 0$, there is a non-trivial solution of the partial differential equation, say $X(x) = A_0$, where A_0 is an arbitrary constant.

Throughout this solution, we reuse the letters A and B for different arbitrary constants.

(d) If $\mu = -k^2$, where k is a positive constant, then the general solution of the equation for $X(x)$ is of the form

$$X(x) = A\cos(kx) + B\sin(kx),$$

where A and B are arbitrary constants. The derivative of this solution is

$$X'(x) = -Ak\sin(kx) + Bk\cos(kx).$$

The boundary condition $X'(0) = 0$ gives $Bk = 0$, so we must have $B = 0$, allowing us to write

$$X'(x) = -Ak\sin(kx).$$

The boundary condition $X'(L) = 0$ then gives either $Ak = 0$ or $\sin(kL) = 0$. Because $k \neq 0$, the first possibility gives $A = 0$. This leads to the trivial solution $c(x,t) = 0$, and is neglected. The remaining possibility gives $k = n\pi/L$, where n is any integer. The allowed values of $\mu = -k^2$ are therefore

$$\mu = -\frac{n^2\pi^2}{L^2}.$$

The value $n = 0$ can be excluded because it gives $\mu = 0$, and we are currently assuming $\mu < 0$. The corresponding solutions for $X(x)$ are

$$X(x) = A_n \cos\left(\frac{n\pi x}{L}\right).$$

In both this equation and the equation for μ, the values for n can be restricted to the positive integers $n = 1, 2, 3, \ldots$, because $-n$ gives exactly the same solutions and values as $+n$.

(e) Since $\mu = -n^2\pi^2/L^2$, the differential equation satisfied by $T(t)$ is

$$T'(t) = -\frac{n^2\pi^2 D}{L^2}\,T(t),$$

with $n = 1, 2, 3, \ldots$. The general solution is of the form

$$T_n(t) = \alpha_n \exp\left(-\frac{n^2\pi^2 Dt}{L^2}\right) \quad (n = 1, 2, 3, \ldots),$$

where α_n is an arbitrary constant.

(f) Assimilating the two arbitrary constants into one (i.e. replacing $A_n\alpha_n$ with C_n), the family of product solutions is

$$c_n(x,t) = C_n \cos\left(\frac{n\pi x}{L}\right) \exp\left(-\frac{n^2\pi^2 Dt}{L^2}\right) \quad (n = 1, 2, 3, \ldots),$$

supplemented by the constant solution

$$c_0(x,t) = C_0.$$

The general solution is therefore of the form

$$c(x,t) = C_0 + \sum_{n=1}^{\infty} C_n \cos\left(\frac{n\pi x}{L}\right) \exp\left(-\frac{n^2\pi^2 Dt}{L^2}\right).$$

(g) Setting $t = 0$ in the general solution, the initial condition $c(x,0) = f(x)$ gives

$$c(x,0) = C_0 + \sum_{n=1}^{\infty} C_n \cos\left(\frac{n\pi x}{L}\right) = f(x).$$

The coefficients C_0 and C_n can therefore be recognised as the coefficients that appear in the cosine Fourier series for $f(x)$ over the interval $0 \le x \le L$. We can therefore find these coefficients by using the *even* periodic extension of $f(x)$.

Note carefully why the *even* periodic extension of $f(x)$ is needed here.

Assuming that this has fundamental period $2L$, and using equations (39) and (40) from Unit 11, we get

$$C_0 = \frac{2}{2L}\int_0^L f(x)\,dx, \quad C_n = \frac{4}{2L}\int_0^L f(x)\cos\left(\frac{n\pi x}{L}\right)dx.$$

3 Modelling heat flow

3.1 The heat equation

It turns out that the diffusion equation (36) also describes the conduction of heat. In a one-dimensional situation, if $\theta(x,t)$ is the temperature at position x and time t, then it is often valid to assume that

$$\frac{\partial\theta}{\partial t} = D\,\frac{\partial^2\theta}{\partial x^2}. \tag{46}$$

This is identical to the diffusion equation but, in this context, the equation is called the **heat equation**, and the constant D is called the **thermal diffusivity**. We do not derive the heat equation here, but the link with diffusion is intriguing, so we make a few remarks about it.

Some authors use a different symbol, such as α, for the thermal diffusivity.

If you apply heat to a metal object, such as a saucepan, by holding it over a flame, then its temperature increases at the point where the heat is supplied. If you remove the pan from the flame, then the heat spreads out so that hot parts become cooler but other parts of the pan become warmer. Although heat is not a substance (it is a form of energy), it does behave in many respects like a fluid, diffusing from hot regions to cooler ones.

The quantities of concentration and flux density, which you met in the context of molecular diffusion, have analogues in the context of heat flow. Temperature can be modelled as being proportional to the heat energy density, which is analogous to concentration, and there is a heat flux density that is analogous to the flux density for molecules. Moreover, it is reasonable to assume that the heat energy density obeys an equation of continuity, and by analogy with Fick's law of diffusion, the heat flux density obeys the equation

$$\text{heat flux density} \propto -\text{temperature gradient}, \tag{47}$$

which is called **Fourier's law**. When all these things are put together, it is possible to justify equation (46), following much the same route as used for the diffusion equation in Section 2.

At a broader level, the analogy is that the conduction of heat occurs via many random steps that involve the transport of heat energy, while molecular diffusion occurs via many random steps that involve the transport of matter.

3.2 Heat flow in rods

We consider a straight thin metal rod of length L with a uniform cross-section. The position of a point on the rod is measured by the distance x from one end. The temperature at this point is θ, which is a function of position x and time t. Two different problems are introduced in this subsection, and then solved in the subsections that follow.

A thermally insulated rod

The simplest case occurs when the only direction of heat flow is along the rod. In this case the temperature satisfies the one-dimensional heat equation

$$\frac{\partial \theta}{\partial t} = D\,\frac{\partial^2 \theta}{\partial x^2}. \qquad \text{(Eq. 46)}$$

Usually, a heated metal rod loses heat to its surroundings, so that heat flows out of its sides as well as along its length. This flow of heat to the surroundings can be stopped (or at least greatly reduced) by covering the rod with a thermal insulating layer (an example is the layer of foam plastic that is used to cover water pipes in houses). For this reason we will refer to the case where the temperature satisfies equation (46) as the **insulated rod**.

The boundary conditions depend on what happens at the ends of the rod. There are two important cases.

- If the ends of the rod are insulated, then no heat can enter or leave them. Fourier's law (47) then implies that the temperature gradient $\partial\theta/\partial x$ is equal to zero at both ends of the rod. This applies at all times of interest, so in mathematical notation, the boundary conditions are

$$\frac{\partial \theta}{\partial x}(0,t) = 0, \quad \frac{\partial \theta}{\partial x}(L,t) = 0, \quad t > 0. \qquad (48)$$

- If the ends of the rod are in contact with a body that is at a fixed temperature θ_0, then the boundary conditions are

$$\theta(0,t) = \theta_0, \quad \theta(L,t) = \theta_0, \quad t > 0. \qquad (49)$$

  In this case, heat may flow from the centre of the rod and out through its ends, even though these are maintained at a fixed temperature. Hence, by Fourier's law, the temperature gradient $\partial\theta/\partial x$ need not be equal to zero at the ends of the rod.

In addition to the boundary conditions, we need an initial condition. Typically, this is given by a function $f(x)$ that describes the initial distribution of temperature along the rod at time $t = 0$. This initial condition is written as

$$\theta(x,0) = f(x), \quad 0 \le x \le L. \qquad (50)$$

Exercise 10

Show that the function

$$\theta(x,t) = \sin\left(\frac{\pi x}{L}\right)\exp\left(-\frac{\pi^2 Dt}{L^2}\right)$$

satisfies the heat equation (46) and boundary conditions (49) if $\theta_0 = 0$.

A convecting rod

The second case that we will discuss is that of a rod that is not thermally insulated, but is surrounded by air. In this case, heat is not only conducted along the rod, but also lost from its sides. Loss of heat from the sides of the rod occurs through a process called **convection**. In this process, as the air around the rod is heated, it expands and rises, so air currents are set up. The process of convection differs from the process of conduction that leads to the heat equation (just as the process of stirring a liquid differs from diffusion). It is therefore not surprising that heat loss due to convection is not described by the heat equation.

Convection is a complex process, but if a hot body at a uniform temperature θ is surrounded by cooler air at temperature θ_{air}, the rate of drop of temperature of the body can be modelled as being proportional to the temperature difference $\theta - \theta_{\text{air}}$. We therefore write

This relationship was introduced by Newton and is sometimes called **Newton's law of cooling**.

$$\left[\frac{d\theta}{dt}\right]_{\text{convection}} = -\gamma(\theta - \theta_{\text{air}}), \qquad (51)$$

where γ is a positive constant that depends on the body's size, shape and composition. The initial minus sign on the right-hand side shows that the temperature of the body is decreasing.

In equation (51), the body is assumed to have a single temperature at each moment in time. In general, the temperature of a convecting rod depends on both position x and time t. We can take account of both conduction along the rod and convection away from the sides of the rod by adding a term $-\gamma(\theta - \theta_{\text{air}})$ to the right-hand side of the diffusion equation (46), where $\theta = \theta(x,t)$ is now a function of position as well as time, and θ_{air} is a constant. We therefore take the partial differential equation for a convecting rod to be

$$\frac{\partial\theta}{\partial t} = D\,\frac{\partial^2\theta}{\partial x^2} - \gamma(\theta - \theta_{\text{air}}). \qquad (52)$$

The boundary and initial conditions are as for an insulated rod.

Exercise 11

Write down the initial condition describing the temperature distribution if the central third of a rod with ends at $x = 0$ and $x = L$ is initially heated to a temperature θ_1 while the remainder of the rod is at the temperature θ_0.

We now solve the two types of problem in turn: first the insulated rod in Subsection 3.3, and then the convecting rod in Subsection 3.4.

3.3 The insulated rod problem solved

This subsection uses Procedure 1 (the method of separation of variables) to solve the heat equation for the insulated rod problem introduced in Subsection 3.2.

In our model, the temperatures at the ends of the rod are zero ($\theta(0,t) = \theta(L,t) = 0$ in appropriate units), and we suppose that the initial temperature of the rod at $t = 0$ is given by a function $f(x)$ that is very similar to the initial displacement function for the taut string problem considered in Section 1 (equation (31)). This initial temperature distribution is sketched in Figure 16.

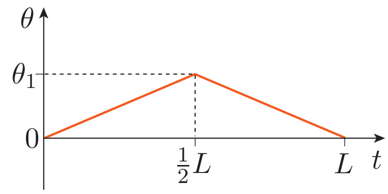


Figure 16 Initial temperature distribution for the insulated rod problem

In mathematical terms, the model is

$$\frac{\partial^2 \theta}{\partial x^2} = \frac{1}{D}\frac{\partial \theta}{\partial t}, \tag{53}$$

subject to boundary conditions

$$\theta(0,t) = \theta(L,t) = 0, \quad t \geq 0, \tag{54}$$

and initial condition

$$\theta(x,0) = f(x) = \begin{cases} \dfrac{2\theta_1}{L}x & \text{for } 0 < x \leq \frac{1}{2}L, \\ \dfrac{2\theta_1}{L}(L-x) & \text{for } \frac{1}{2}L < x < L. \end{cases} \tag{55}$$

You will see that the solution of this problem is simplified by having $\theta = 0$ at the ends of the rod. This might seem strange because there are many different temperature scales, and a temperature of zero degrees Fahrenheit, for example, has no great physical significance. In fact, the choice of boundary conditions in equation (54) is made purely for mathematical convenience. You will see later how our solution can be adapted to cover any fixed temperatures at the ends of the rod.

- **Step 1 Prepare a product solution**

  We prepare to separate the variables by writing

  $$\theta(x,t) = X(x)\,T(t), \tag{56}$$

  and finding the relevant partial derivatives:

  $$\frac{\partial^2 \theta}{\partial x^2} = X''T, \tag{57}$$

  $$\frac{\partial \theta}{\partial t} = XT'. \tag{58}$$

- **Step 2 Separate the variables**

  To get separate ordinary differential equations for $X(x)$ and $T(t)$, we substitute the formulas for the partial derivatives into the partial differential equation, and rearrange.

Substituting equations (57) and (58) into equation (53) gives

$$X''T = \frac{1}{D}XT'.$$

Dividing by XT then gives

$$\frac{X''}{X} = \frac{1}{D}\frac{T'}{T}. \tag{59}$$

The left-hand side is a function of the variable x alone, and the right-hand side is a function of the variable t alone, so both are equal to the same separation constant μ. Thus the single equation (59) gives us the pair of equations

$$X'' - \mu X = 0, \tag{60}$$

$$T' - D\mu T = 0. \tag{61}$$

- **Step 3 Prepare the boundary conditions**

  To find the boundary conditions for $X(x)$, we write $\theta(x,t) = X(x)\,T(t)$, substitute in $x = 0$ and $x = L$, and then use the given boundary conditions for $\theta(x,t)$. This gives $X(0)\,T(t) = X(L)\,T(t) = 0$ for $t \geq 0$, and hence

  $$X(0) = X(L) = 0. \tag{62}$$

- **Step 4 Find the functions $X_n(x)$**

  The differential equation (60) for X, and its boundary conditions (62), are the same as in Subsection 1.2, so we need not repeat the arguments. You have seen that a non-trivial solution occurs only if the constant μ is negative. Hence, as before, we replace μ by $-k^2$.

  As before, k must take one of the values $k_n = n\pi/L$, where n is an integer. As explained in Section 1, n can be restricted further to the positive integers, $n = 1, 2, 3, \ldots$. The allowed values of the separation constant are $\mu_n = -k_n^2 = -n^2\pi^2/L^2$, and each of these values corresponds to a solution

  $$X_n(x) = B_n \sin(k_n x) = B_n \sin\left(\frac{n\pi x}{L}\right), \quad n = 1, 2, 3, \ldots, \tag{63}$$

  where B_n is an arbitrary constant.

- **Step 5 Find the functions $T_n(x)$**

  The function $T(t)$ satisfies the differential equation $T' = D\mu T$, where μ is restricted to the values $\mu_n = -k_n^2$. We therefore need to solve the first-order differential equation

  $$T_n'(t) = -Dk_n^2 T,$$

  which has general solution

  $$T_n(t) = \alpha_n \exp(-Dk_n^2 t) = \alpha_n \exp\left(-\frac{n^2\pi^2 Dt}{L^2}\right), \tag{64}$$

  where α_n is an arbitrary constant and $n = 1, 2, 3, \ldots$.

- **Step 6 Construct the general solution**

  By combining $X_n(t)$ and $T_n(t)$, we obtain a family of product solutions $X_n(x)\,T_n(t)$ that satisfy the heat equation (53) and its associated boundary conditions (54). This family is

$$\theta_n(x,t) = C_n \sin\left(\frac{n\pi x}{L}\right) \exp\left(-\frac{n^2\pi^2 Dt}{L^2}\right), \quad n = 1, 2, 3, \ldots, \tag{65}$$

  where $C_n = B_n\alpha_n$ is obtained by combining the arbitrary constants B_n and α_n. The *general solution* is an infinite linear combination of members from this family:

$$\theta(x,t) = \sum_{n=1}^{\infty} C_n \sin\left(\frac{n\pi x}{L}\right) \exp\left(-\frac{n^2\pi^2 Dt}{L^2}\right). \tag{66}$$

- **Step 7 Apply the initial condition**

  Setting $t = 0$ in equation (66) gives

$$\theta(x,0) = \sum_{n=1}^{\infty} C_n \sin\left(\frac{n\pi x}{L}\right).$$

  The function $f(x)$ used in initial condition (55) is essentially the same as that used in Section 1, hence we arrive at the same values for the coefficients C_n. The required particular solution is therefore

$$\begin{aligned}\theta(x,t) = \frac{8\theta_1}{\pi^2}\Bigg[&\sin\left(\frac{\pi x}{L}\right) \exp\left(-\frac{\pi^2 Dt}{L^2}\right) \\ &- \frac{1}{9}\sin\left(\frac{3\pi x}{L}\right) \exp\left(-\frac{9\pi^2 Dt}{L^2}\right) \\ &+ \frac{1}{25}\sin\left(\frac{5\pi x}{L}\right) \exp\left(-\frac{25\pi^2 Dt}{L^2}\right) - \cdots\Bigg].\end{aligned} \tag{67}$$

As promised earlier, let us now see how to adjust this solution to cover the case where the ends of the rod are maintained at a constant non-zero temperature $\theta_0 \neq 0$, i.e. where the boundary conditions are

$$\theta(0,t) = \theta(L,t) = \theta_0, \quad t \geq 0. \tag{68}$$

The trick is to notice that the constant function $\theta(x,t) = \theta_0$ satisfies the heat equation (53). This is because all of its partial derivatives are equal to zero, so substituting into the heat equation gives $0 = 0$. If we ignore the boundary conditions for the moment, then the principle of superposition tells us that any linear combination of solutions of the heat equation is also a solution. So we can add the constant solution θ_0 to the solution obtained in equation (66) to get another solution of the heat equation:

$$\theta(x,t) = \theta_0 + \sum_{n=1}^{\infty} C_n \sin\left(\frac{n\pi x}{L}\right) \exp\left(-\frac{n^2\pi^2 Dt}{L^2}\right). \tag{69}$$

If we substitute $x = 0$ or $x = L$ into this expression, we already know that all the terms in the summation will give zero (because they satisfy the boundary conditions $\theta(0,t) = \theta(L,t) = 0$).

It follows that $\theta(x,t)$ in equation (69) satisfies the new boundary conditions in equation (68). In fact, it is the *general solution* of the heat equation subject to these boundary conditions.

Exercise 12

Consider the heat equation

$$\frac{\partial^2\theta}{\partial x^2} = \frac{1}{D}\frac{\partial\theta}{\partial t},$$

subject to the boundary conditions

$$\theta(0,t) = \theta(L,t) = \theta_0, \quad t \geq 0,$$

where $\theta_0 \neq 0$. Explain how you would obtain the particular solution that satisfies the initial condition

$$\theta(x,0) = f(x), \quad 0 \leq x \leq L,$$

where $f(x)$ is a given function that is equal to θ_0 at $x = 0$ and $x = L$.

Exercise 13

Consider the heat equation

$$\frac{\partial^2\theta}{\partial x^2} = \frac{1}{D}\frac{\partial\theta}{\partial t},$$

subject to boundary conditions

$$\theta(0,t) = \theta_0, \quad \theta(L,t) = \theta_L, \quad t \geq 0,$$

These boundary conditions model the situation where the ends of the rod are kept at two different fixed temperatures.

where θ_0 and θ_L are non-zero constants, and initial condition

$$\theta(x,0) = f(x), \quad 0 < x < L,$$

for some function $f(x)$.

(a) Show that the function

$$\theta(x,t) = \frac{L-x}{L}\,\theta_0 + \frac{x}{L}\,\theta_L$$

satisfies the differential equation and the boundary conditions.

(b) Write down the general solution of the partial differential equation subject to the boundary conditions.

(c) Explain how you would go on to obtain a solution that also satisfies the initial condition.

3.4 The convecting rod problem solved

In this subsection, we again use Procedure 1 (the method of separation of variables). This time, we solve the heat equation for the convecting rod problem, sharing the solution between text and exercises.

We suppose that the ambient temperature of the air, and the temperature at the ends of the rod, are equal to zero (in appropriate units). The initial

condition is the same as for the insulated rod. In mathematical terms, the problem is

$$\frac{\partial \theta}{\partial t} = D \frac{\partial^2 \theta}{\partial x^2} - \gamma\theta, \tag{70}$$

where $D > 0$, subject to the boundary conditions

$$\theta(0,t) = \theta(L,t) = 0, \quad t \geq 0, \tag{71}$$

and the initial condition

$$\theta(x,0) = \begin{cases} \dfrac{2\theta_1}{L} x & \text{for } 0 < x \leq \frac{1}{2}L, \\ \dfrac{2\theta_1}{L}(L-x) & \text{for } \frac{1}{2}L < x \leq L. \end{cases} \tag{72}$$

Exercise 14

Carry out Steps 1 and 2 of Procedure 1 for the convecting rod problem, as follows.

(a) Prepare a product solution for substitution into equation (70).

(b) Separate the variables.

The ordinary differential equations derived in Exercise 14 are

$$X'' - \mu X = 0,$$
$$T' = (D\mu - \gamma)T.$$

Steps 3 and 4 in Procedure 1 tell us to prepare the boundary conditions for $X(x)$ and to solve the differential equation for $X(x)$ subject to them. Applying the given boundary conditions to the product function $\theta(x,t) = X(x)\,T(t)$ gives $X(0)\,T(t) = X(L)\,T(t) = 0$, so the boundary conditions for $X(x)$ are

$$X(0) = 0 \quad \text{and} \quad X(L) = 0.$$

These are the same boundary conditions as those used for an insulated rod (in Subsection 3.2) and for a string (in Section 1). The same arguments apply, so we do not repeat them here – although you would need to when answering an assignment question!

In brief, the conclusions are as follows. In order to get non-trivial solutions that satisfy the boundary conditions, μ must be negative. Writing $\mu = -k^2$, the boundary conditions require that k takes one of the values $k_n = n\pi/L$, where n is an integer. The corresponding solutions for $X(x)$ are

$$X_n(x) = B_n \sin\left(\frac{n\pi x}{L}\right), \quad n = 1, 2, 3, \ldots,$$

where B_n is an arbitrary constant. The values of n have been restricted to the positive integers because $n = 0$ gives the trivial solution and $-n$ gives the same solution as $+n$.

Exercise 15

Step 5 in Procedure 1 asks us to solve the differential equation for $T(t)$, to find the functions $T_n(t)$ that accompany $X_n(x)$ in the product solutions. Carry out this step using the differential equation for T obtained above.

In Step 6 of Procedure 1 we combine the solutions for $X_n(x)$ and $T_n(t)$, to obtain a family of product solutions of equation (70) subject to boundary conditions (71):

$$\begin{aligned}\theta_n(x,t) &= C_n \sin\left(\frac{n\pi x}{L}\right)\exp\left[-\left(D\frac{n^2\pi^2}{L^2}+\gamma\right)t\right]\\ &= C_n \sin\left(\frac{n\pi x}{L}\right)\exp\left[-D\frac{n^2\pi^2 t}{L^2}\right]e^{-\gamma t}, \quad n=1,2,3,\ldots,\end{aligned}$$

where we have combined the arbitrary constants B_n and α_n to give $C_n = B_n\alpha_n$. The general solution of the partial differential equation, satisfying the associated boundary conditions, is then given by the infinite sum

$$\theta(x,t) = e^{-\gamma t}\sum_{n=1}^{\infty} C_n \sin\left(\frac{n\pi x}{L}\right)\exp\left[-D\frac{n^2\pi^2 t}{L^2}\right].$$

The factor $e^{-\gamma t}$ has been brought outside the summation because it is independent of n.

Finally, Step 7 of Procedure 1 asks us to apply the given initial condition. Setting $t=0$ in the expression for the general solution gives

$$\theta(x,0) = \sum_{n=1}^{\infty} C_n \sin\left(\frac{n\pi x}{L}\right),$$

and we can equate this to the given initial temperature distribution $f(x)$, given in equation (72). The computation of the Fourier coefficients is exactly the same as in the previous cases (see, for example, equation (67)).We conclude that the required particular solution is

$$\begin{aligned}\theta(x,t) = \frac{8\theta_1}{\pi^2}\,e^{-\gamma t}\Bigg[&\sin\left(\frac{\pi x}{L}\right)\exp\left(-\frac{\pi^2 Dt}{L^2}\right)\\ &-\frac{1}{9}\sin\left(\frac{3\pi x}{L}\right)\exp\left(-\frac{9\pi^2 Dt}{L^2}\right)\\ &+\frac{1}{25}\sin\left(\frac{5\pi x}{L}\right)\exp\left(-\frac{25\pi^2 Dt}{L^2}\right)-\cdots\Bigg].\end{aligned} \tag{73}$$

This is the same as the solution for the insulated rod except for the $e^{-\gamma t}$ factor, which ensures that the convecting rod cools more quickly towards the ambient zero temperature than the insulated rod.

4 Taking a broader view

This final section will not be assessed in continuous assessment or in the exam, but you should read it, especially if you plan to study further modules in the physical sciences or applied mathematics.

This section differs in style from the rest of the unit because it takes a light-touch approach, emphasising concepts rather than problem solving. After a brief review of some areas of science that use partial differential equations, we consider solutions of the wave equation and the diffusion equation that apply when the region of interest has no boundaries, or has boundaries that are so far away that they do not influence the solutions. Under these circumstances, there are alternative methods of solution, not based on the method of separation of variables.

4.1 The importance of partial differential equations

Partial differential equations have a vast range of applications. This is partly because many fundamental laws of physics are expressed directly in terms of them. So when physical theories are applied to other subjects, such as climate science, astrophysics or physiology, partial differential equations are often used.

Partial differential equations in action

- The laws of electromagnetism are expressed as a system of equations called *Maxwell's equations*. These lead to a three-dimensional version of the wave equation that describes light and similar waves. Electrostatic phenomena are also described using a partial differential equation called *Poisson's equation*.
- Atoms and molecules are best described using quantum mechanics. The description often involves using a partial differential equation called the *Schrödinger equation* that is closely related to both the wave equation and the diffusion equation.
- A vast range of phenomena involve the effects of numerous small random motions, and are described by variants of the diffusion equation, including the *Black–Scholes equation* for price fluctuations.
- The motion of fluids is described by non-linear partial differential equations called the *Navier–Stokes equations*. These equations are used in oceanography and weather science.

- The most successful theory of gravity, called *general relativity*, is expressed as a system of non-linear partial differential equations. These equations are used to model the expansion of the Universe and the collapse of black holes.

A basic classification of partial differential equations distinguishes between linear and non-linear equations. The fundamental partial differential equations of electromagnetism and quantum mechanics are linear, and so is the diffusion equation. But the Navier–Stokes equations of fluid mechanics are non-linear, and so are the equations of general relativity.

This distinction is important because non-linear partial differential equations are usually very hard to solve using mathematical analysis alone. The solutions may be too complex to allow description by manageable mathematical formulas, and investigations using computer programs may be the only practical approach. An example is given in Figure 17, which shows a solution of the Navier–Stokes equations for the flow of a gas above a hot surface.

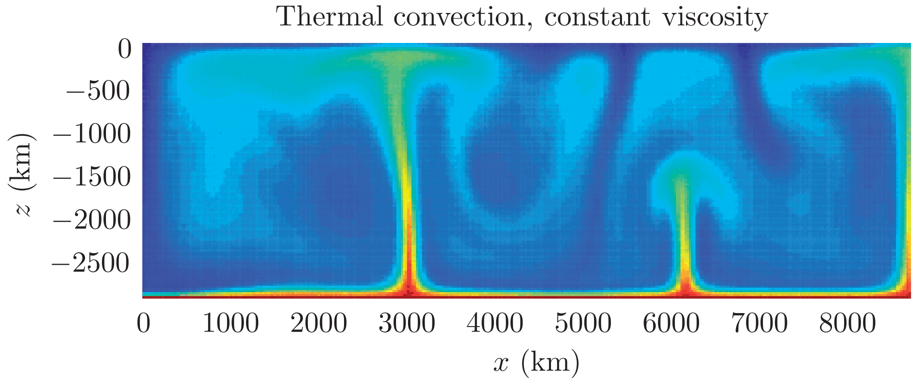


Figure 17 A computer-generated colour-coded image of the temperature of air above a hot surface, with 'plumes' of hot air rising at apparently random positions

4.2 Travelling wave solutions of the wave equation

When discussing waves on a string earlier, we kept the ends of the string clamped. This introduced boundary conditions that restricted the family of product solutions obtained by the method of separation of variables.

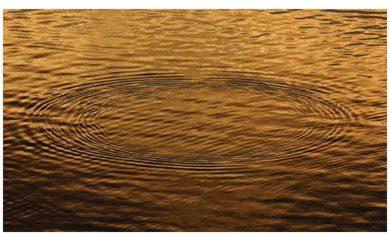


Figure 18 Wave ripples produced by dropping a stone into a lake

However, there are many situations where boundary conditions are irrelevant. When a stone is dropped into the middle of a large lake, the ripples that spread out do not depend strongly on the details of the lake's shoreline (Figure 18). It therefore makes sense to consider solutions of the wave equation that apply in the absence of boundary conditions. In the context of a string, we simply ignore the ends of the string and treat it as if it were infinitely long. This may seem rather artificial for a string, but it is often a good way of thinking about the propagation of light, sound and many other types of wave.

In the absence of boundary conditions, a proposed solution need only satisfy the wave equation. One function that does so is

$$u(x,t) = A\sin[k(x-ct)], \tag{74}$$

where A and k are constants, and c is the wave speed that appears in the wave equation. You can check this by calculating the relevant partial derivatives and substituting into the wave equation.

Exercise 16

Check that the function in equation (74) satisfies the wave equation

$$\frac{\partial^2 u}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} = 0.$$

Exercise 16 showed that the function $A\sin[k(x-ct)]$ is a solution of the wave equation for any values of k and A. This function varies sinusoidally, and gives a train of wave crests and troughs that move through space as time progresses (Figure 19). The distance between two successive wave crests is the **wavelength** of this sinusoidal wave. The wavelength λ is related to the constant k in equation (74) by $k\lambda = 2\pi$, so $\lambda = 2\pi/k$.

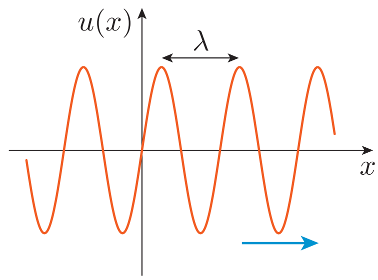


Figure 19 A sinusoidal wave solution travelling in the positive x-direction

Suppose that at time t, a particular crest is at position x. At a slightly later time $t+\Delta t$, the same crest has moved to position $x+\Delta x$. The function $A\sin[k(x-ct)]$ must take the same value at both these instants, so

$$A\sin[k(x+\Delta x - c(t+\Delta t))] = A\sin[k(x-ct)].$$

We need to satisfy this equation in a way that ensures that $\Delta x \to 0$ as $\Delta t \to 0$. This is achieved by taking

$$\Delta x = c\,\Delta t.$$

The constant c is positive, so $\Delta x > 0$ when $\Delta t > 0$, and we see that the wave crest (and every other part of the wave) moves in the positive x-direction at the constant speed $\Delta x/\Delta t = c$. This is why the constant c in the wave equation is called the *wave speed*. A disturbance that travels in this way is called a **travelling wave** solution of the wave equation.

Instead of $u(x,t) = A\sin[k(x-ct)]$, we could consider $u(x,t) = A\sin[k(x+ct)]$: the same steps show that this is another travelling wave solution of the wave equation. In this case, the wave moves in the negative x-direction with speed c. We could also replace $A\sin[k(x-ct)]$ by $A\cos[k(x\pm ct)]$ and find that these too are solutions.

In fact, the crucial feature for a travelling wave solution of the wave equation is that x and t should appear in one of the combinations $x-ct$ or $x+ct$. If we take any reasonable function, and work out the partial derivatives, we find that $f(x-ct)$ and $f(x+ct)$ are solutions of the wave equation, provided that the function f can be differentiated twice.

To check that this is true, note that if $u(x,t) = f(x-ct)$, then

$$\frac{\partial u}{\partial x} = f'(x-ct), \quad \frac{\partial u}{\partial t} = -cf'(x-ct),$$
$$\frac{\partial^2 u}{\partial x^2} = f''(x-ct), \quad \frac{\partial^2 u}{\partial t^2} = c^2 f''(x-ct).$$

Hence

$$\frac{\partial^2 u}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} = f''(x-ct) - \frac{1}{c^2}c^2 f''(x-ct) = 0,$$

showing that $f(x-ct)$ satisfies the wave equation. A similar argument applies to $f(x+ct)$.

In general, if f and g are two functions that can be differentiated twice, then the following function is a solution of the wave equation:

$$u(x,t) = f(x-ct) + g(x+ct). \tag{75}$$

This is known as **d'Alembert's solution** of the wave equation. It is the general solution of the wave equation without boundary conditions. It consists of two travelling waves, moving in opposite directions, but one or other of these waves may be missing in particular cases. There is an immense amount of freedom built into this general solution, which can be restricted by considering particular initial conditions.

A solution like $f(x-ct)$ describes a pulse of disturbance that travels at constant speed, unchanged in shape, as in Figure 20. The fact that the pulse travels unchanged in shape is a consequence of our assumption that the wave speed c is a constant. There are other types of wave for which this is not true, and whose pulses broaden out as they travel. These are described by partial differential equations that are more complicated than the wave equation of this unit. Some examples are given in the box below.

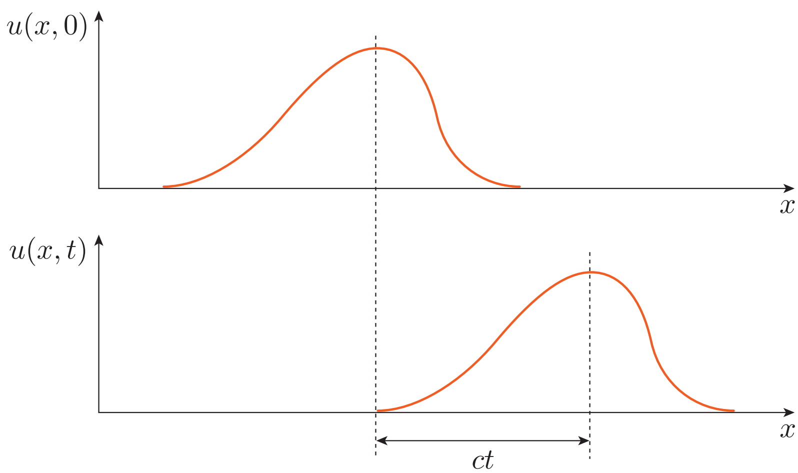


Figure 20 A pulse travels at constant speed, unchanged in shape

Waves are everywhere

A wave is a disturbance of some kind that either forms standing waves or propagates through space as time progresses. The partial differential equations satisfied by waves are called *wave equations*, although they may differ from equation (3).

- **Electromagnetic waves** are disturbances of electric and magnetic fields. In empty space, they satisfy a three-dimensional version of equation (3). This equation has sinusoidal solutions with definite wavelengths, and the wavelength determines the name given to the wave. Radio waves have very long wavelengths; as the wavelength decreases, we progress through infrared radiation, microwaves, visible light, ultraviolet radiation, X-rays and gamma rays. In a vacuum, all these waves have the same wave speed, $c = 3.0 \times 10^8\,\mathrm{m\,s^{-1}}$, which is called the speed of light.
- **Sound waves** are disturbances of the pressure in a gas or liquid. They also obey a three-dimensional version of equation (3). In air, sound waves have a speed that is roughly $330\,\mathrm{m\,s^{-1}}$.
- **Water waves** on the surface of the sea are very familiar. Their wave speed is not a constant, but depends on the wavelength.
- **Quantum-mechanical waves** arise in the most fundamental theory of nature, *quantum mechanics*. The relevant wave equation is called the *Schrödinger equation*, which differs from equation (3) because it involves complex numbers and only the first-order partial derivative with respect to time.

4.3 Point-source solutions of the diffusion equation

Finally, let us briefly consider the phenomenon of diffusion in a region that is large enough for its boundaries to be irrelevant. If you inject a drop of dye into the centre of a large tank of still water, the dye molecules gradually spread out from their starting point: this is the essence of the phenomenon of diffusion.

We can imagine an idealised one-dimensional situation in which all the molecules start out at $x = 0$ at $t = 0$. Because all the molecules start from a single point, this initial condition is referred to as a **point source**. Figure 21 shows the spread of concentrations that arise from this source at a series of later times. Of course, the spreading out is accompanied by a reduction in concentration at the injection point, $x = 0$.

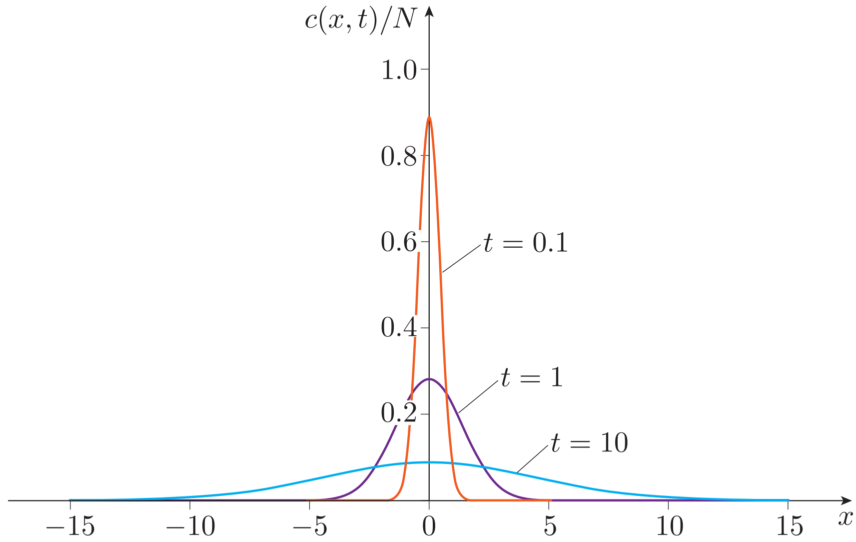


Figure 21 The concentration resulting from a point source at $x = 0$ injected at time $t = 0$. (The diffusion coefficient D has been taken as 1.)

The function that describes this spreading out of concentration turns out to be

$$c(x,t) = \frac{N}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right) \quad (t > 0), \tag{76}$$

where N is a constant. Although there are powerful techniques for deriving this function, they are not discussed here. However, you can verify for yourself that this function does satisfy the diffusion equation.

Exercise 17

Show that the function $c(x,t)$ in equation (76) satisfies

$$\frac{\partial c}{\partial x} = -\frac{x}{2Dt}\,c \quad \text{and} \quad \frac{\partial c}{\partial t} = \left(\frac{x^2}{4Dt^2} - \frac{1}{2t}\right)c.$$

Then carry out a further partial differentiation to show that $c(x,t)$ satisfies the diffusion equation.

Because it describes the diffusion of a point source at $x = 0$, released at $t = 0$, the function in equation (76) is called a **point-source solution** of the diffusion equation.

If the particles had been released from a different point, say $x = s$, at $t = 0$, then the corresponding point-source solution would be of the form

$$c(x,t) = \frac{N_1}{\sqrt{4\pi Dt}} \exp\left[-\frac{(x-s)^2}{4Dt}\right],$$

where N_1 is another constant.

It turns out (although again we do not give the details) that the general solution of the diffusion equation without boundaries can be expressed as

$$c(x,t) = \frac{1}{\sqrt{4\pi Dt}} \int_{\infty}^{\infty} \exp\left[-\frac{(x-s)^2}{4Dt}\right] c_0(s)\, du,$$

where $c(x,t)$ satisfies the initial condition $c(x,0) = c_0(x)$. Thinking of this integral as a sort of 'continuous sum', you can see that it can be interpreted as a linear superposition of point-source solutions. This is not too surprising, since we know that the diffusion equation is linear and satisfies the principle of superposition.

Learning outcomes

After studying this unit, you should be able to do the following.

- Understand how the wave and diffusion/heat partial differential equations are used to model certain systems.
- Use the method of separation of variables to find families of product solutions for the wave equation, diffusion equation and similar linear homogeneous second-order partial differential equations, subject to simple boundary conditions.
- Construct the general solution of a partial differential equation from a family of product solutions.
- Find the values of the coefficients in the general solution of a partial differential equation by using given initial conditions to determine the coefficients of a Fourier series.

Solutions to exercises

Solution to Exercise 1

The partial derivatives are

$$\frac{\partial u}{\partial x} = Ak\cos(kx)\sin(kct), \quad \frac{\partial u}{\partial t} = Akc\sin(kx)\cos(kct),$$
$$\frac{\partial^2 u}{\partial x^2} = -Ak^2\sin(kx)\sin(kct), \quad \frac{\partial^2 u}{\partial t^2} = -Ak^2c^2\sin(kx)\sin(kct),$$

so

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2}.$$

The function does satisfy the wave equation.

Solution to Exercise 2

The displacement at $t = 0$ is

$$u(x, 0) = A\sin(kx)\sin(0) = 0.$$

The velocity at position x and time t is

$$\frac{\partial u}{\partial t} = Akc\sin(kx)\cos(kct),$$

so the velocity at position x and time $t = 0$ is

$$\frac{\partial u}{\partial t}(x, 0) = Akc\sin(kx).$$

Solution to Exercise 3

The initial displacement has two linear sections.

The left-hand section has slope $d/(L/3) = 3d/L$ and has the value $u = 0$ at $x = 0$. It is described by the function $u(x) = (3d/L)x$.

The right-hand section has slope $-d/(2L/3) = -3d/2L$ and has the value $u = 0$ at $x = L$. It is described by a linear function of the form

$$u(x) = -\frac{3d}{2L}x + C,$$

where C is a constant. Setting $u(L) = 0$ gives $C = 3d/2$, so the right-hand section is described by the function

$$u(x) = \frac{3d}{2} - \frac{3d}{2L}x = \frac{3d}{2L}(L - x).$$

The initial condition for the shape of the string is therefore

$$u(x, 0) = \begin{cases} \dfrac{3d}{L}x & \text{for } 0 \le x \le \frac{1}{3}L, \\[2ex] \dfrac{3d}{2L}(L - x) & \text{for } \frac{1}{3}L < x \le L. \end{cases}$$

You can check that both parts of this expression give $u(x, 0) = d$ at $x = L/3$.

The condition for the initial shape of the string is supplemented by the condition that a plucked string is released from rest:

$$\frac{\partial u}{\partial t}(x,0)=0,\quad 0\le x\le L.$$

Solution to Exercise 4

The function under consideration is

$$u(x,t)=\sin\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi ct}{L}\right).$$

The boundary conditions are satisfied since

$$u(0,t)=\sin 0\cos\left(\frac{\pi ct}{L}\right)=0,\quad u(L,t)=\sin\pi\cos\left(\frac{\pi ct}{L}\right)=0.$$

The initial condition is satisfied since

$$\frac{\partial u}{\partial t}(x,t)=-\frac{\pi c}{L}\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{\pi ct}{L}\right),$$

so at $t=0$,

$$\frac{\partial u}{\partial t}(x,0)=-\frac{\pi c}{L}\sin\left(\frac{\pi x}{L}\right)\sin(0)=0.$$

Solution to Exercise 5

Substituting $u(x,t)=X(x)\,T(t)$ into the partial differential equation gives

$$X\,\frac{d^2T}{dt^2}=T\,\frac{d^4X}{dx^4}.$$

Dividing by XT and equating both sides to the same separation constant μ, we get

$$\frac{1}{T}\,\frac{d^2T}{dt^2}=\mu=\frac{1}{X}\,\frac{d^4X}{dx^4},$$

and this leads to the ordinary differential equations

$$\frac{d^2T}{dt^2}=\mu T,\quad \frac{d^4X}{dx^4}=\mu X.$$

Solution to Exercise 6

Substituting $u(x,t)=X(x)\,T(t)$ into the partial differential equation gives

$$X\,\frac{dT}{dt}=T\left[\frac{d}{dx}(xX)+\frac{d^2X}{dx^2}\right].$$

Dividing by XT and equating both sides to the same separation constant μ, we get

$$\frac{1}{T}\,\frac{dT}{dt}=\mu=\frac{1}{X}\left[\frac{d}{dx}(xX)+\frac{d^2X}{dx^2}\right],$$

and this leads to the ordinary differential equations

$$\frac{dT}{dt}=\mu T,\quad \frac{d}{dx}(xX)+\frac{d^2X}{dx^2}=\mu X.$$

Solution to Exercise 7

When $u(x,t) = a_1\, u_1(x,t) + a_2\, u_2(x,t)$,

$$\begin{aligned}\frac{\partial^2 u}{\partial x^2} &= \frac{\partial^2}{\partial x^2}(a_1 u_1 + a_2 u_2)\\ &= a_1 \frac{\partial^2 u_1}{\partial x^2} + a_2 \frac{\partial^2 u_2}{\partial x^2}\\ &= a_1 \frac{1}{c^2}\frac{\partial^2 u_1}{\partial t^2} + a_2 \frac{1}{c^2}\frac{\partial^2 u_2}{\partial t^2}\\ &= \frac{1}{c^2}\frac{\partial^2}{\partial t^2}(a_1 u_1 + a_2 u_2) = \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2},\end{aligned}$$

so the linear combination satisfies the wave equation.

The given boundary conditions lead to

$$\begin{aligned}u(0,t) &= a_1\, u_1(0,t) + a_2\, u_2(0,t) = 0,\\ u(L,t) &= a_1\, u_1(L,t) + a_2\, u_2(L,t) = 0,\end{aligned}$$

Hence the linear combination $u = a_1 u_1 + a_2 u_2$ satisfies the wave equation *and* the given boundary conditions.

Solution to Exercise 8

From equation (35), the velocity at $t = 0$ is

$$v(x) = \frac{\partial u}{\partial t}(x,0) = \sum_{n=1}^{\infty} \left(\frac{n\pi c}{L}\right) B_n \sin\left(\frac{n\pi x}{L}\right) \cos(0).$$

If the Fourier coefficients of $v(x)$ are C_n, then

$$B_n = \frac{L}{n\pi c} C_n, \quad n = 1, 2, 3, \ldots.$$

Solution to Exercise 9

Step 1 Setting $u(x,t) = X(x)\,T(t)$, the required partial derivatives are

For brevity, primes are used to denote derivatives.

$$\frac{\partial^2 u}{\partial x^2} = X''T, \quad \frac{\partial^2 u}{\partial t^2} = XT''.$$

Step 2 Substituting into the partial differential equation and dividing by XT gives

$$\frac{X''}{X} + \frac{T''}{T} = 0,$$

from which it follows that

$$\frac{X''}{X} = -\frac{T''}{T}.$$

Both sides of the equation must be equal to the same constant μ, giving

$$\frac{X''}{X} = \mu \quad \text{and} \quad -\frac{T''}{T} = \mu,$$

or equivalently,

$$X'' - \mu X = 0 \quad \text{and} \quad T'' + \mu T = 0.$$

Step 3 The boundary conditions become $X(0) = X(1) = 0$.

Step 4 Arguing as in Subsection 1.2, only negative μ gives a non-trivial solution for X. Hence we can write $\mu = -k^2$, and the differential equation for X becomes

$$X'' + k^2 X = 0.$$

This equation has the general solution

$$X(x) = C\cos(kx) + D\sin(kx),$$

where C and D are arbitrary constants. In order to satisfy the boundary condition at $x = 0$, we must have $C = 0$. Then, to satisfy the boundary condition at $x = 1$, we must have $k = n\pi$ for some integer n. So there is a family of solutions

$$X_n(x) = D_n \sin(n\pi x), \quad n = 1, 2, 3, \ldots,$$

where we have dropped the value $n = 0$ because it gives the trivial solution $X(x) = 0$, and we have dropped negative values of n because $-n$ gives the same solution as $+n$ (since D_n is an arbitrary constant).

Step 5 With $\mu = -k^2$, the differential equation for T becomes

$$T'' - k^2 T = 0.$$

This equation has the general solution

$$T(t) = Ae^{kt} + Be^{-kt}.$$

Using the allowed values for k, the allowed solutions are

$$T_n(t) = A_n e^{n\pi t} + B_n e^{-n\pi t}, \quad n = 1, 2, 3, \ldots.$$

Step 6 Replacing $D_n A_n$ and $D_n B_n$ by α_n and β_n, respectively, the required family of product solutions is

$$u_n(x,t) = \sin(n\pi x)\,(\alpha_n e^{n\pi t} + \beta_n e^{-n\pi t}), \quad n = 1, 2, 3, \ldots,$$

where α_n and β_n are arbitrary constants. The general solution is therefore

$$u(x,t) = \sum_{n=1}^{\infty} \sin(n\pi x)\,(\alpha_n e^{n\pi t} + \beta_n e^{-n\pi t}).$$

Solution to Exercise 10

We have

$$\frac{\partial\theta}{\partial x} = \frac{\pi}{L}\cos\left(\frac{\pi x}{L}\right)\exp\left(-\frac{\pi^2 Dt}{L^2}\right),$$

so

$$\frac{\partial^2\theta}{\partial x^2} = -\frac{\pi^2}{L^2}\sin\left(\frac{\pi x}{L}\right)\exp\left(-\frac{\pi^2 Dt}{L^2}\right) = -\frac{\pi^2}{L^2}\,\theta(x,t).$$

Also,

$$\frac{\partial\theta}{\partial t} = -\frac{\pi^2 D}{L^2}\sin\left(\frac{\pi x}{L}\right)\exp\left(-\frac{\pi^2 Dt}{L^2}\right) = -\frac{\pi^2 D}{L^2}\,\theta(x,t).$$

Hence
$$\frac{1}{D}\frac{\partial\theta}{\partial t} = -\frac{\pi^2}{L^2}\,\theta(x,t) = \frac{\partial^2\theta}{\partial x^2},$$
showing that equation (46) is satisfied.

At the ends of the rod,
$$\theta(0,t) = \exp\left(-\frac{\pi^2 Dt}{L^2}\right)\sin 0 = 0, \quad \theta(L,t) = \exp\left(-\frac{\pi^2 Dt}{L^2}\right)\sin\pi = 0,$$
so the boundary conditions are satisfied if $\theta_0 = 0$.

Solution to Exercise 11

The initial condition is
$$\theta(x,0) = \begin{cases} \theta_0 & \text{for } 0 \le x < \frac{1}{3}L, \\ \theta_1 & \text{for } \frac{1}{3}L \le x \le \frac{2}{3}L, \\ \theta_0 & \text{for } \frac{2}{3}L < x \le L. \end{cases}$$

Solution to Exercise 12

The general solution satisfying the given boundary conditions is
$$\theta(x,t) = \theta_0 + \sum_{n=1}^{\infty} C_n \sin\left(\frac{n\pi x}{L}\right)\exp\left(-\frac{n^2\pi^2 Dt}{L^2}\right).$$
Setting $t = 0$, we obtain
$$\theta(x,0) = \theta_0 + \sum_{n=1}^{\infty} C_n \sin\left(\frac{n\pi x}{L}\right).$$
So to satisfy the initial condition $\theta(x,0) = f(x)$, we need to obtain the C_n from the Fourier sine series coefficients of the function $f(x) - \theta_0$. Substituting these coefficients into equation (69) then gives the required solution.

Solution to Exercise 13

(a) For
$$\theta(x,t) = \frac{L-x}{L}\,\theta_0 + \frac{x}{L}\,\theta_L,$$
we have
$$\frac{\partial^2\theta}{\partial x^2} = 0 \quad \text{and} \quad \frac{\partial\theta}{\partial t} = 0,$$
so the heat equation reduces to $0 = 0$ and is satisfied.

At $x = 0$, we have
$$\theta(0,t) = \frac{L-0}{L}\,\theta_0 + 0 = \theta_0,$$
and at $x = L$, we have
$$\theta(L,t) = \frac{L-L}{L}\,\theta_0 + \frac{L}{L}\,\theta_L = \theta_L,$$
so the boundary conditions are satisfied.

(b) The general solution takes the form

$$\theta(x,t) = \frac{L-x}{L}\,\theta_0 + \frac{x}{L}\,\theta_L + \sum_{n=1}^{\infty} C_n \sin\left(\frac{n\pi x}{L}\right) \exp\left(-\frac{n^2\pi^2 Dt}{L^2}\right), \qquad (*)$$

where the C_n are arbitrary constants, and the sum on the right satisfies the same differential equation, but with boundary conditions corresponding to zero temperature at both ends of the rod. By the principle of superposition, the general solution $(*)$ satisfies the partial differential equation. It also satisfies the given boundary conditions. This is because substituting in $x = 0$ gives θ_0 from the terms outside the sum and zero from the sum. Similarly, substituting in $x = L$ gives θ_L from the terms outside the sum and zero from the sum.

(c) To find a solution that satisfies the initial condition, we set $t = 0$ in equation $(*)$. This gives

$$\theta(x,0) = \frac{L-x}{L}\,\theta_0 + \frac{x}{L}\,\theta_L + \sum_{n=1}^{\infty} C_n \sin\left(\frac{n\pi x}{L}\right).$$

So to satisfy $\theta(x,0) = f(x)$, we need to obtain the C_n as the Fourier sine series coefficients of the function

$$g(x) = f(x) - (L-x)\theta_0/L - x\theta_L/L.$$

Substituting these into equation $(*)$ gives the required result.

The Fourier sine series coefficients are found using the odd periodic extension of $g(x)$.

Solution to Exercise 14

(a) Set $\theta(x,t) = X(x)\,T(t)$. Then

$$\frac{\partial^2\theta}{\partial x^2} = X''T \quad \text{and} \quad \frac{\partial\theta}{\partial t} = XT'.$$

(b) Equation (70) becomes

$$XT' = DX''T - \gamma XT,$$

and dividing by XT gives

$$\frac{T'}{T} = D\frac{X''}{X} - \gamma.$$

Thinking a step ahead, we soon need to solve a differential equation for $X(x)$. To make this equation as simple as possible, we make a rearrangement to get

$$\frac{X''}{X} = \frac{1}{D}\left(\frac{T'}{T} + \gamma\right).$$

The left-hand side is a function of x alone, and the right-hand side is function of t alone, so both must be equal to the same constant μ (the separation constant). We therefore get the ordinary differential equations

$$X'' - \mu X = 0, \quad T' = (D\mu - \gamma)T.$$

Solution to Exercise 15

The relevant differential equation is

$$T' = (D\mu - \gamma)T.$$

For a particular value of n, this takes the form

$$T' = -(Dk_n^2 + \gamma)T,$$

which has general solution

$$\begin{aligned} T_n(t) &= \alpha_n \exp(-(Dk_n^2 + \gamma)t) \\ &= \alpha_n \exp\left[-\left(D\frac{n^2\pi^2}{L^2} + \gamma\right)t\right], \quad n = 1, 2, 3, \ldots, \end{aligned}$$

where α_n is an arbitrary constant.

Solution to Exercise 16

The required partial derivatives are calculated using the chain rule:

$$\begin{aligned} \frac{\partial u}{\partial x} &= kA\cos[k(x - ct)], \quad \frac{\partial u}{\partial t} = -kcA\cos[k(x - ct)], \\ \frac{\partial^2 u}{\partial x^2} &= -k^2 A\sin[k(x - ct)], \quad \frac{\partial^2 u}{\partial t^2} = -k^2c^2 A\sin[k(x - ct)]. \end{aligned}$$

Substituting these partial derivatives into the wave equation gives

$$\frac{\partial^2 u}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} = -k^2 A\sin[k(x - ct)] + \frac{1}{c^2}\left(k^2c^2 A\sin[k(x - ct)]\right) = 0,$$

as required. So we see that $A\sin[k(x - ct)]$ is a solution of the wave equation, for any values of k and A.

Solution to Exercise 17

The chain rule of differentiation gives

$$\frac{\partial c}{\partial x} = \frac{N}{\sqrt{4\pi Dt}}\exp(-x^2/4Dt) \times \left(\frac{-2x}{4Dt}\right) = -\frac{x}{2Dt}\,c.$$

Also,

$$\begin{aligned} \frac{\partial c}{\partial t} &= -\frac{1}{2}t^{-3/2}\frac{N}{\sqrt{4\pi D}}\exp(-x^2/4Dt) + \frac{N}{\sqrt{4\pi Dt}}\exp(-x^2/4Dt) \times \left(\frac{x^2}{4Dt^2}\right) \\ &= -\frac{1}{2t}\,c + \frac{x^2}{4Dt^2}\,c = \left(\frac{x^2}{4Dt^2} - \frac{1}{2t}\right)c. \end{aligned}$$

Partially differentiating $\partial c/\partial x$ with respect to x again, we get

$$\frac{\partial^2 c}{\partial x^2} = \frac{x^2}{4D^2t^2}\,c - \frac{1}{2Dt}\,c = \left(\frac{x^2}{4D^2t^2} - \frac{1}{2Dt}\right)c.$$

Taking all the derivatives in the diffusion equation onto the left-hand side, and substituting in the above results, then gives

$$\frac{\partial c}{\partial t} - D\frac{\partial^2 c}{\partial x^2} = \left(\frac{x^2}{4Dt^2} - \frac{1}{2t}\right)c - D\left(\frac{x^2}{4D^2t^2} - \frac{1}{2Dt}\right)c = 0,$$

as required.

Acknowledgements

Grateful acknowledgement is made to the following sources:

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